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MASS TRANSFER ANALYSIS IN REVERSE OSMOSIS OPERATION. (9) PROGRESS REPORT. 1 MARCH - DECEMBER 1968

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Progress Report on Grant WP-00968-02
"Mass Transfer Analysis in Reverse Osmosis Operation"
For the Period of March 1, 1968 - December, 1968

Details of illustrations in this document may be better studied on microfiche.

I. INTRODUCTION

The purpose of this report is to present a summary of the major achievement of the work performed during the period March 1968 to December 1968 in connection with the research Grant WP-00968-02, "Mass Transfer Analysis in Reverse Osmosis Operation", and the significance and relevance of these results to the use of R.O. in waste water treatment. In addition, a brief description of the work to be carried in the coming period (i.e. March 1, 1969 - February 1970) will also be given.

The objective of this program is to carry out an analysis on the mass transfer characteristics of reverse osmosis, especially in connection with its application on waste water treatment. The feasibility study of using R.O. for waste water treatment was first made by General Dynamics in 1963. More recent works, including those in various demonstrating plants, have clearly demonstrated the potential superiority of R.O. in waste treatment.

The specific aim of this work is to formulate a general procedure of design of R.O. process. That is to say, to obtain a rational method which can be used in estimating the process capacity from operating conditions and membrane parameters. The extensive use of numerical analysis in this work may give the unintended impression that the study carried out under this grant is of the nature basic and academic, while in reality the ultimate objective of this work is to provide practical design information for R.O. process.

For the purpose of clarification, a brief description on the mass transfer problem associated with R.O. process will be given. The separation process in a reverse osmosis operation is effected through the use of a semi-permeable membrane which allows the passage of water but not dissolve salt. Ordinarily speaking, if a salt solution and pure water are placed on either side of the membrane, water

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will flow from the water side to the solution because of the exertion of osmotic pressure. However, if the pressure exerted on the side of salt solution is greater than that of osmotic pressure, the flow of water will be reversed. That is, water will be transferred from the salt solution side to the pure water side, and this is known as reverse osmosis.

Many theories have been proposed to explain the mechanism of permeation of water across a semi-permeable membrane. For engineering purposes, the simple phenomenological law is found to be applicable:

$$V_w = A \left[\Delta p - \pi_{os} \right] \tag{1}$$

where V_w is the linear velocity of water permeation across membrane, Δp is pressure difference across membrane (i.e. the pressure difference between salt solution side and pure water side), and π_{os} is the osmotic pressure. For a given kind of salt solution, the osmotic pressure is a function of salt concentration. The proportional constant, A, is known as membrane constant.

The capacity of a reverse osmosis plant is given as,

$$Q(\text{volume of water recovered per unit time}) = \int_0^S V_w \cdot dS \tag{2}$$

where S is the area of membrane sheet.

It is obvious that Q can be evaluated if V_w is known. The evaluation of V_w, according to Equation (1), requires the knowledge of salt concentration at the surface of the membrane since the osmotic pressure, π_{os} is to be evaluated corresponding to this surface concentration.

The main mass transfer problem in reverse osmosis process is to determine this salt concentration at membrane surface. In this regard, one may point out that the permeation of water across membrane implies the bulk movement of salt solution toward the membrane surface. However, since the membrane is impermeable to salt, the salt concentration accumulates at membrane surface. From the principal of conservation

of material, the concentration build-up shall be such that it provides a molecular diffusion flux away from the membrane of sufficient magnitude to compensate the convective salt flux due to bulk motion. The salt concentration at membrane surface, therefore, greatly exceeds the bulk concentration and, furthermore, it increases along the downstream direction. The phenomenon that salt concentration is higher at membrane surface is commonly referred to as concentration polarization. The determination of concentration polarization and the subsequent determination of quantitative relationship between the capacity and operating conditions represents the major effort of our program.

II. SUMMARY OF WORKS PERFORMED DURING THE PAST YEAR

Three major studies were completed. These are:

(1) It has been long recognized that mass transfer rate is enhanced if the flow is turbulent. Consequently, one may expect substantial reduction of concentration polarization effect which is inherent in any R.O. process, by operating at turbulent conditions. With the objective in mind, a numerical analysis was carried out considering reverse osmosis in turbulent flow with flat membrane duct. The results of this work clearly indicates the substantial reduction of concentration polarization. This work has been accepted for publication and a copy of the manuscript is attached (see Appendix A).

It may be in order to make a few comments on the possible use of turbulent flow condition in R.O. process for waste water treatment. The development of R.O. process has been mostly linked with desalination effort and the use of turbulent flow condition has been greatly ruled out because of the high pressure requirement in treating sea water (this is due to the relative high salt concentration in sea water). For the case of waste water, the relative low salt concentration makes it desirable to consider the use of turbulent condition for the advantage of reducing concentration

polarization, which is amply demonstrated in this work. In this regard, it may become necessary to require R.O. hardware developed specifically for waste water instead of adopting existing equipment which is primarily designed for sea water. It should be added that the difference of these two requirements could result not only in a variation in operating conditions (laminar vs turbulent) but also different geometrical configurations as well as membrane characteristics (for example, in the case of waste water one may use a type of membrane with high water flux but also with poor salt rejection).

(2) Reverse Osmosis of Multicomponent System

Most of the previous studies on the convection diffusion process in reverse osmosis has been confined to one-solute system. The justification of this assumption is that in the case of sea water, sodium chloride is the predominant species of solute and, therefore, represents the only solute which needs to be considered in the mass transfer analysis. The assumption obviously is not applicable to the case of waste water and, furthermore, it overlooks an important aspect that one of the frequently encountered difficulties in membrane process is the saturation and precipitation of salts onto membrane even though the overall concentration level of these salts is very small. A number of membrane plants treating brackish water have found the necessity of adding pretreatment facilities during the course of actual operation.

Because of these considerations, it is necessary to include all species of solute in the considering of mass transfer in R.O. process. An analysis of this type was performed during this period and the result of this work is scheduled for publication in the forthcoming issue of Desalination. A copy of the preprint is included in Appendix B.

The interesting result of this work is the finding, that even though the concentration polarization effect has been found to be strongly dependent

upon the presence of other species of salt, the mass transfer characteristics in terms of Sherwood number (i.e. mass transfer coefficient for a given salt remains relatively unchanged). Furthermore, the Sherwood number for various solutes is found to be proportional to the third power of their respective Schmidt number. These findings enable the establishment of a simplified procedure for prediction of concentration polarization in R.O. process, which will be discussed in later sections.

(3) The Establishment of a Simplified Procedure for Prediction of Concentration Polarization in R.O. Process

As stated before, the overall objective of this research work is to obtain the quantitative information on the concentration polarization in a reverse osmosis system. The general procedure involved in this endeavor requires the solution of the appropriate diffusion equations. As demonstrated in the attached articles, this usually requires rather extensive mathematical manipulations and numerical computations which make it impractical for design engineers to use. Furthermore, the large number of parameters present in a given situation and the many possible variations in the process itself precludes the possibility of carrying out extensive computation to establish "a master plot".

In view of these difficulties, attempts were made during the past year in developing a simple procedure which can be conveniently used in predicting the concentration polarization phenomenon. This effort turned out to be successive. In Appendix C, a description of this method is presented.

The successful development of this simplified procedure, in our opinion, constitutes a major achievement. Specifically, its significance can be stated as follows:

(a) The relative simple procedure (i.e. Equation (37) of Appendix C) makes it possible for design engineers to consider in detail the

concentration polarization phenomena. It also enables a more accurate calculation of required plant size for a given situation. The solution of Equation (37) in Appendix C can be programmed as a subroutine and can be incorporated with the excellent general computer program for waste water treatment, which is being developed by Mr. Robert Smith of Cincinnati Water Research Laboratory.

(b) It enables the prediction of concentration polarization of all species of salts present in the waste water stream. With this information available, the saturation of a given salt (a solute) can be determined. Consequently, one can predict more accurately as to the necessity of pretreatment of feed streams.

(c) The procedure developed here can be used in conjunction with actual operation data to determine the relative performance efficiency of the various hardwares. For example, one can obtain "membrane constant" from actual plant data in conjunction with this procedure, and by observing its change with time, one can obtain quantitative information about the useful life span of the respective membranes.

(d) The establishment of this procedure make it possible to make simulations as well as optimization studies of R.O. process in a simple straightforward manner.

III. PROPOSED WORK DURING THE COMING YEAR

The following studies will be carried out during the last year of the project period.

(1) Effect of Organic Contaminants

In the previous studies, only inorganic salt is considered. For the case of waste water, the consideration of organic contaminants is of equal importance. Mass transfer analysis, therefore, will be made to include the consideration of organic matters and the possible interaction between organic and inorganic substances will be focused.

(2) Effect of Membrane Fouling

One of the serious problems encountered in using R.O. treating waste water has been the fouling of membranes which result in the reduction of water flux. In order to obtain a realistic subject model for R.O., it is necessary to incorporate this phenomenon into our analysis. This means that one should consider the mass transfer process as an unsteady-state one instead of the steady-state assumption. Such an analysis will be made.

(3) Evaluation of Available Experimental Results in Terms of Analytical Model

Aerojet-General Corporation is currently conducting pilot plant work on the treatment of waste water from a secondary treatment plant under contract with FWPCA. Through the courtesy of Mr. Robert Smith of Cincinnati Laboratory, some of their monthly progress reports have become available to this Grantee. It appears that the results of this pilot plant work can be analyzed in terms of the study carried out in our project. The objectives of this phase of proposed work are:

(a) To determine the adequacy of the theoretical analysis for the description of R.O. operation in waste water treatment.

(b) To determine, at least, in a semi-quantitative way the effect of fouling and compaction on membrane characteristics in terms of the reduction of membrane constant as a function of time.

It should also be pointed out that for carrying out this work additional information on the dimensions and configurations of the membrane units are required. For this reason, permission to use their experimental results have to be obtained from Aerojet-General.

(4) Mass Transfer Analysis of Other Configurations

All the mass transfer analyses carried out in our work are confined to two types of configurations, tubular and plate. Several other types of configurations have also been employed in membrane fabrication, notably Dupont's hollow fiber and the Roga membrane module (spiral tube) of Gulf General Atomic. In order to provide some qualitative basic for performance evaluation of these types of membrane configuration, mass transfer analyses will be carried out in the proposed investigation.

A FINITE DIFFERENCE SOLUTION FOR REVERSE OSMOSIS IN TURBULENT FLOW

by

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ABSTRACT

A finite difference solution for reverse osmosis in turbulent flow is presented. The case of a flat duct made of two parallel semi-permeable membranes is considered. The pertinent diffusion equation with the eddy diffusivity based on Deissler's expression is solved using a two-step linearized finite difference scheme, taking into account the nonlinear effect due to the varying water flux across membrane along the axial direction. Numerical results relating concentration polarization, water flux, Sherwood number water recovery ratio and operating conditions are given for a variety of cases.

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INTRODUCTION

A number of investigations have been reported in the literature in recent years relating the performance of reverse osmosis systems with system configurations and operating variables. The earlier work of Merten (7) described the concentration polarization phenomenon in reverse osmosis operation based on one-dimensional diffusion and film model. A more exact analysis was performed by Sherwood, Brian, Fisher and Dresner (9). Based on Berman's expression for the velocity profile, the two-dimensional diffusion equation was solved in a manner similar to that of the classical Graetz-Nusselt problem assuming constant longitudinal water flux across the membrane. It was pointed out in a subsequent study (5) that this rather arbitrary assumption of constant water flux can be removed and a perturbation solution valid for short axial length was obtained. A finite difference solution for the same problem has also been carried out (1). For a more general two-dimensional case, Gill, Tien and Lee (6) obtained an asymptotic solution to the diffusion equation, in which the velocity profile within the concentration boundary layer was approximated by a linear expression because of the relatively high value of the Schmidt number of the water-salt system. The approximate method of integral solution has also been found useful for the solution of reverse osmosis problems and studies on the simultaneous development of velocity and concentration profiles for a number of cases has already been made (10,11). Although different assumptions have been made in these studies, the flow conditions of the works cited above (5,6,9,10,11) were assumed to be laminar.

The assumption of laminar flow for reverse osmosis process is well understood since almost all of these earlier studies were concerned primarily with desalination of sea water. For sea water with an average salt concentration of 3.5%, the osmotic pressure is around 350 psi. In terms of the membranes available today as well as those anticipated in the near future, the operating pressure for a reverse osmosis system should be about 1000 psi in order to have reasonable production capacity. In view of this relatively high operating pressure and also owing to the fact that the distance between adjacent membranes is extremely narrow, the flow within a membrane duct would necessarily be laminar.

The same consideration, however, does not remain valid if fairly dilute systems are to be treated such as the treatment and renovation of waste water. In turbulent flow, mass transfer rates are usually enhanced by the added eddy diffusion. Consequently, concentration polarization in the turbulent flow case would be somewhat less severe and so does its distribution effect. Turbulent flow in reverse osmosis may very well be more advantageous even with added pressure drops.

For reverse osmosis in turbulent flow, Dresner (4) obtained the following expression:

$$\Gamma = c_w^+ - 1 = 25 \left(\frac{v_w}{u_B}\right) \left[N_{Re_E}\right]^{1/4} \left[N_{Sc}\right]^{2/3} \qquad \text{(I-1)}$$

Similar expressions have also been given by Sherwood and co-workers (8). The above expression, undoubtedly valuable in a qualitative sense, does not yield precise information required for a better understanding of the process because of the substantial difference between the basic assumptions used and the actual operating conditions. Consequently, great caution must be exercised for the proper interpretation of the results of these expressions. For example, an average value of v_w needs to be defined since in practice v_w does not remain constant but decreases along the axial direction.

The object of this investigation is to present a detailed analysis on the mass transfer characteristics of reverse osmosis in turbulent flow. Specifically, the system considered is that of parallel membrane sheets with salt solution flowing in between. A finite difference solution for the pertinent diffusion equation using Deissler's expression for eddy diffusivity is obtained using a two-step linearized finite difference scheme. The use of finite difference is primarily due to the fact that comparatively fewer assumptions are involved in this method. Furthermore, the finite difference method is applicable to both large and small longitudinal distances and, therefore, less restrictive as compared with the series solution employed for the laminar case.

FORMULATION OF PROBLEM

A schematic description of the physical problem is given in Figure 1. Salt solution with an initial concentration c_I and osmotic pressure $(P_{os})_I$ under pressure is forced through a flat duct whose walls are made of parallel semi-permeable membranes. The distances between the membranes is 2b. The flow is assumed to be turbulent.

Because of symmetry, it is only necessary to consider half of the conduit. The pertinent diffusion equation, in dimensionless form, can be written as follows:

$$u^+ b^+ \frac{\partial c^+}{\partial x^+} + \left[N_{Re_W}\right]\left[N_{Re}\right] v^+ \frac{\partial c^+}{\partial z^+} = \left[N_{Re_I}\right] \frac{\partial}{\partial z^+}\left(\Lambda \frac{\partial c^+}{\partial z^+}\right) \qquad \text{(II-1)}$$

where

$$\Lambda = \frac{1}{N_{Sc}} + \frac{\epsilon}{\nu} \qquad \text{(II-2)}$$

$$N_{Re_W} = \frac{bV_{W_o}}{\nu} \qquad \text{(II-3a)}$$

$$N_{Re_I} = \frac{bU_o}{\nu} \qquad \text{(II-3b)}$$

$$b^+ = \frac{b}{\nu}\sqrt{\frac{\tau_w}{\rho}} \qquad \text{(II-4)}$$

The boundary conditions are:

$$c^+ = 1 \text{ at } x^+ = 0,\ 0 \leq z^+ \leq 1 \qquad \text{(II-5)}$$

$$\frac{\partial c^+}{\partial z^+} = 0 \text{ at } z^+ = 1,\ x^+ > 0 \qquad \text{(II-6)}$$

$$-\left(\frac{\partial c^+}{\partial z^+}\right) = \left[N_{Re_w}\right]\left[N_{Sc}\right] v^+ c^+ \text{ at } z^+ = 0,\ x^+ > 0 \qquad \text{(II-7)}$$

where N_{Sc} is the Schmidt number and is taken to be 560. In Equation (II-7), it is implicitly assumed that the membrane rejects the salt completely.

The water flux, v_w, across the membrane is given by the phenomenological law

$$v_w = A\left[\Delta P - (P_{os})\right] \qquad \text{(II-8)}$$

where A is the membrane constant, ΔP is the pressure drop across the membrane and P_{os} is the osmotic pressure. Assuming that the concentration variation of osmotic pressure is linear, one has,

$$v_w = A(\Delta P)\left[1 - \frac{(P_{os})_I}{\Delta P}\,\frac{c_w}{c_I}\right] \qquad \text{(II-9)}$$

The dimensionless quantity, v_w^+, is then

$$v_w^+ = \frac{v_w}{v_{w_o}} = \frac{1}{1-B_2} - \frac{B_2}{1-B_2}\,c_w^+ \qquad \text{(II-10)}$$

and

$$B_2 = (P_{os})_I/\Delta P \qquad \text{(II-11)}$$

The fraction of water recovered, Q^+, may be obtained by integrating the wall velocity with respect to the axial distance. Q^+ is given by the following equation:

$$q^+ = \left[N_{Re_w} \right] \int_o^{x^+} v_w^+ \, dx^+ \qquad \text{(II-12)}$$

For the solution of Equation (II-1), it is necessary to describe the velocity field as well as the eddy diffusivity which is part of the term, A. It is assumed that because the permeation velocity, v_w, is of much smaller magnitude as compared to the axial velocity, u, its effect may be ignored and the velocity expressions given by Deissler (3) may be used. These are:

$$u^+ = \int_o^{y^+} \frac{dy^+}{1 + (0.124)^2 \, u^+ y^+ \left[1 - \exp\left(- 0.124^2 \, u^+ y^+ \right) \right]} \qquad \text{(II-13a)}$$

$$y^+ < 26$$

and

$$u^+ = u_1^+ + \frac{1}{0.36} \ln \left(\frac{y^+}{26} \right), \quad y^+ > 26 \qquad \text{(II-13b)}$$

where u_1^+ is taken to be the value of u^+ at $y^+ = 26$. The transverse velocity component, v^+, is assumed to be independent of z^+ and equal to the value of v_w^+. The eddy diffusivity term, $\frac{\epsilon}{\nu}$, is:

$$\frac{\epsilon}{\nu} = (0.124)^2 \, u^+ y^+ \left[1 - \exp\left(- 0.124^2 \, u^+ y^+ \right) \right], \quad y^+ < 26 \qquad \text{(II-14a)}$$

$$\frac{\epsilon}{\nu} = 0.36 \, y^+ \left(1 - \frac{y^+}{b^+} \right), \quad y^+ > 26 \qquad \text{(II-14b)}$$

Equations (II-1) together with Equations (II-13a,b) - (II-14a,b) and the boundary conditions of Equations (II-5) - (II-7), give a complete description of the physical problem and the solution of this system of equations represents the main object of the present investigation. It should be mentioned that the parameter, b^+, present in Equation (II-1) varies along the axial direction because of the continuous permeation of pure water across the membrane. The quantity, b^+, can be related to the equivalent Reynolds number, N_{Re_E}, as follows:

$$b^+ = \frac{N_{Re_E}}{4}\sqrt{\frac{f}{2}} \qquad \text{(II-15)}$$

Furthermore, the fraction factor, f, can be expressed in terms of N_{Re_E} by the well known Blasius equation,

$$f = 0.079\left[N_{Re_E}\right]^{-1/4} \qquad \text{(II-16)}$$

Since water is being withdrawn from the system, N_{Re_E} decreases continuously. As a consequence, the parameter, b^+, the velocity profile, u^+, as well as the eddy diffusivity expressions all vary along the axial direction. The manner in which these variations are being accounted for will be described in the following section.

NUMERICAL SOLUTION

A two-step linearized finite difference scheme which has been proved successful in the past (1) is used for the solution of Equation (II-1) with the boundary conditions of Equations (II-5) - (II-7). A brief description of the procedure is given as follows.

The first step of the computation scheme consists in obtaining an approximate concentration profile for the advance longitudinal position in a marching process, i.e. to obtain concentration value at the i+1st x^+ position using the concentration values at the preceding mesh points. For this purpose, a corresponding difference equation of Equation (II-1) is obtained by approximating the various derivatives as follows:

$$\frac{\partial c^+}{\partial x^+} = \frac{c^+_{i+1,j} - c^+_{i,j}}{\Delta x^+} \qquad \text{(III-1)}$$

$$\frac{\partial c^+}{\partial u^+} = \frac{c^+_{i+1,j+1} - c^+_{i+1,j-1}}{2\Delta u^+} \qquad \text{(III-2)}$$

$$\frac{\partial}{\partial z^+}\left(\Lambda \frac{\partial c^+}{\partial z^+}\right) = \frac{\Lambda_{j+1/2}\, c^+_{i+1,\,j+1} - (\Lambda_{j+1/2} + \Lambda_{j-1/2})\, c^+_{i+1,j} + \Lambda_{j-1/2}\, c^+_{i+1,\,j-1}}{(\Delta z^+)^2} \qquad \text{(III-3)}$$

The mesh network is shown in Figure 2.

Substituting Equations (III-1) - (III-3) into Equation (II-1), after some rearrangement, the following expression is obtained:

$$\left\{\frac{\left[N_{Re_V}\right]\left[N_{Re_I}\right]}{2\Delta z^+} v^+_{i,j} - \frac{\left[N_{Re_I}\right](\Lambda_{j+1/2})}{(\Delta z^+)^2}\right\} c^+_{i+1,\,j+1}$$

$$+\left\{\frac{u^+_{i,j}\, b^+_{i,j}}{\Delta x^+} + \frac{\left[N_{Re_I}\right](\Lambda_{j+1/2} + \Lambda_{j-1/2})}{(\Delta z^+)^2}\right\} c^+_{i+1,j}$$

$$-\left\{\frac{\left[N_{Re_V}\right]\left[N_{Re_I}\right]}{2\Delta z^+} + \frac{\left[N_{Re_I}\right](\Lambda_{j-1/2})}{(\Delta z^+)^2}\right\} c^+_{i+1,\,j-1}$$

$$= \frac{u^+_{i,j}\, b^+_{i,j}}{\Delta x^+} c^+_{i,j} \qquad \text{(III-4)}$$

Equation (III-4) for $j=2,3 \ldots n+1$, yields n equations with $n+2$ unknowns, i.e. $c^+_{i+1,j}$, $j=1,2 \ldots n+1, n+2$ ($j=1$ corresponds to the membrane wall and $j=n+1$ corresponds to the axis of the channel). However, the boundary condition of Equation (II-6) yields $c^+_{i+1,\,n+2} = c^+_{i+1,\,n}$. Also, from Equation (II-7), one has,

$$\left\{\frac{1}{\Delta z^+} - \left[N_{Re_V}\right]\left[N_{Sc}\right] v^+_{i+1,1}\right\} c^+_{i+1,1} - \frac{1}{\Delta z^+} c^+_{i+1,2} = 0 \qquad \text{(III-5)}$$

Here, $v^+_{i+1,1}$ is represented by $v^+_{i,1}$. Thus, one now has $n+1$ equations for the $n+1$ values of concentrations in the channel z^+ position. The system of linear tridiagonal equations is solved by Thomas method (2). This method is equivalent

to plain Gaussian elimination, but is known to avoid the error growth associated with the back solution of the elimination method. The first approximations for $c^{+}_{i+1,1}$ through $c^{+}_{i+1,n+1}$ are thus obtained. Knowing $c^{+}_{i+1,1}$, $\bar{v}^{+}_{i+1,1}$ may be obtained from Equation (II-10). The bar over $v^{+}_{i+1,1}$ indicates that the value is only the first approximation.

The second step involves the formulation of the Crank Nicholson equation for Equation (II-1). This, after some rearrangement, is given as:

$$\left\{ \phi\varepsilon^{n} - \frac{\left[{}^{H}Re_{I} \right] \varepsilon^{n} \left(A_{j+1/2} \right)}{(\Delta z^{+})^{2}} \right\} c^{+}_{i+1,\, j+1}$$

$$+ \left\{ \frac{b^{+}_{i,j}\, u^{+}_{i,j}}{\Delta x^{+}} + \frac{\left[{}^{H}Re_{I} \right] \varepsilon^{n} \left(A_{j+1/2} + A_{j-1/2} \right)}{(\Delta z^{+})^{2}} \right\} c^{+}_{i+1,j}$$

$$- \left\{ \phi\varepsilon^{n} + \frac{\left[{}^{H}Re_{I} \right] \varepsilon^{n} \left(A_{j-1/2} \right)}{(\Delta z^{+})^{2}} \right\} c^{+}_{i+1,\, j-1}$$

$$= \frac{b^{+}_{i,j}\, u^{+}_{i,j}\, c^{+}_{i,j}}{\Delta x^{+}} - \phi G + \frac{H A_{j} \left[{}^{H}Re_{I} \right]}{(\Delta z^{+})^{2}} \qquad \text{(III-6)}$$

where,

$$\phi = \frac{\left[{}^{H}Re_{w} \right] \left[{}^{H}Re_{I} \right]}{2(\Delta z^{+})} \left[\varepsilon^{n} \bar{v}^{+}_{i+1,1} + (1-\varepsilon^{n})\, v^{+}_{x,1} \right] \qquad \text{(III-7)}$$

$$G = (1-\varepsilon^{n}) \left[c^{+}_{i,j+1} - c^{+}_{i,j-1} \right] \qquad \text{(III-8)}$$

$$H = \frac{1-\varepsilon^{n}}{A_{j}} \left[A_{j+1/2}\, c^{+}_{i,j+1} - \left(A_{j+1/2} + A_{j-1/2} \right) c^{+}_{i,j} + A_{j-1/2}\, c^{+}_{i,j-1} \right] \qquad \text{(III-9)}$$

and ε^{n} is the weighting coefficient.

For the present case, a value of $\epsilon^{\circ} = 0.5$ corresponding to Crank Nicholson weighting is used. Similar to the previous step, together with the boundary conditions of Equation (II-6) and Equation (III-5), Equation (III-6) defines n+1 equations with n+1 unknowns, i.e. $c_{i+1,j}$, j=1,2 ... n+1. The value of $v_{i+1,1}$ which appears in Equation (III-5) is approximated by the arithmetic average of $\overline{v^{+}_{i+1,1}}$ and $v^{+}_{i,1}$. This system of n+1 equations in the unknowns, $c^{+}_{i+1,1}$ through $c^{+}_{i+1,\,n+1}$, is then solved and the new concentration values are used to obtain a second approximation of $\overline{v^{+}_{i+1,1}}$, which is then used for another round of calculations. This iteration procedure may be carried out as many times as required, although in almost all cases, three iterations were found adequate. The concentration values from the last iteration performed are taken to be the correct values. This, in turn, are the values used in the calculations for the next advance x^{+} position.

The variation in N_{Re_E} Reynolds number based on equivalent diameter, is given by,

$$\left[N_{Re_E}\right]_{x^{+}} = \left[N_{Re_E}\right]_{I} (1-Q^{*}) \qquad \text{(III-10)}$$

The subscript I refers to the value at the inlet. Q^{*} is obtained from Equation (II-12). Using Equations (II-15) and (II-16), it can be shown that,

$$(b^{*})_{x^{+}} = b^{*}_{I} (1-Q^{*})^{7/3} \qquad \text{(III-11)}$$

b^{*} is calculated for each step and the current value of b^{*} is used in the computation scheme. As pointed out earlier, the velocity and eddy diffusivity expressions involve b^{*} and hence need to be recalculated as b^{*} varies along the longitudinal direction. In the computation performed in this work, these values were recalculated for every five percent increase in the value recovery instead of after every step. This is believed to be a reasonable balance between computer time involved in recalculating the quantities and adherence to the physical model.

RESULTS AND DISCUSSION

The numerical computations were performed on an IBM System/360 digital computer. The following combination of parameters was considered.

$$b_I^+ = 100, 200, 300$$

(These correspond to inlet Reynolds numbers $\left[N_{Re_E}\right]_I$ of 5967, 13175 and 20941, respectively.)

$$N_{Re_w} = 0.006, 0.015$$

$$B_2 = 0, 1/4, 1/3, 1/2$$

($B_2 = 0$ corresponds to very dilute solutions with high operating pressures.) For each set of specified value of b_I^+, N_{Re_w} and B_2, the quantities c_w^+, v_w^+, Q^+, b^+ and N_{Re_E} were calculated as functions of x^+. The results for c_w^+ vs x^+ are presented graphically in Figures 3 to 8. Figures 9 and 10 show typical results for v_w^+ and Q^+ as functions of x^+ for different values of B_2 for $b_I^+ = 200$ and $N_{Re_w} = 0.015$.

It was stated in the previous section that concentration polarization is expected to be reduced with the increased eddy diffusion. The extent of reduction of salt buildup due to the increase of turbulence (in terms of inlet Reynolds number) is clearly indicated in Figures 11 and 12 in which values of c_w^+ were plotted against x^+ with specified values of N_{Re_w} and B_2 for different values of $\left[N_{Re_E}\right]_I$. Because of the presence of the Reynolds number, in the definition of x^+, all the abscissa in these figures were referred to a common value of $\left[N_{Re_E}\right]_I$. The significant reduction of c_w^+ with the increase of inlet Reynolds number becomes quite obvious. Furthermore, the decrease becomes more pronounced with the decrease of the value of B_2 as well as the decrease of N_{Re_w}.

As an example, at $x^+ = 20$ (based on $b_I^+ = 300$), the reduction of the excess salt concentration buildup (defined as $c_w^+ - 1$) is approximately 53% with a 3.5 fold increase of inlet Reynolds number (from 5967 to 20941) for the case of $N_{Re_w} = 0.015$ and $B_2 = 0.5$. The corresponding reduction for the case of $N_{Re_w} = 0.006$ and $B_2 = 0.25$, however, was found to be 82%.

The effect of the parameters B_2 and N_{Re_w} on the production capacity of the reverse osmosis system is indicated in Tables I and II. Based on the definitions given in the nomenclature, it can be seen that the actual amount of pure water produced in proportional to the product of Q^+ and $\left[N_{Re_E}\right]_I$, which was found to be increasing with the increase of $\left[N_{Re_E}\right]_I$. Also, this increase is most pronounced for lower values of B_2 and higher values of N_{Re_w}, which, physically speaking, corresponds to the case of very dilute feed stream operating at relatively high pressures with high capacity membranes. It is interesting to note that these conditions are most likely to be met if reverse osmosis is to be developed as a practical means for treatment of waste water.

The results of this work are also compared with those based on the one-dimensional model. The one-dimensional diffusion equation based on complete salt rejection at the surface of the membrane can be written as:

$$v_w c + (D_B + \varepsilon) \frac{dc}{dy} = 0 \qquad \text{(IV-1)}$$

Using Deissler's expression for eddy diffusivity [Equations (II-14a) and (II-14b)], the following result is obtained after simple integration,

$$\frac{c_w}{c_B} = \exp\left\{ \frac{8.56\, v_w}{u_B} \left[N_{Sc}\right]^{3/4} \sqrt{\frac{2}{f}} \right\} \qquad \text{(IV-2)}$$

A mass balance on the salt indicates that,

$$c_B^+ = \frac{c_B}{c_I} = \frac{1}{1 - Q^+} \qquad \text{(IV-3)}$$

In terms of the dimensionless quantities defined in the present work, Equation (IV-2) may be written as,

$$c_w^+ = \exp\left\{ \frac{(8.96)\left[N_{Re_x}\right]\left[N_{Sc}\right]^{3/4}}{b_I^+} \frac{(\alpha-\beta\, c_w^+)}{(1-Q^+)^{7/8}} - \ln(1-Q^+) \right\} \qquad \text{(IV-4)}$$

where,

$$\alpha = \frac{1}{1-B_2} \qquad \text{(IV-5a)}$$

$$\beta = \alpha B_2 \qquad \text{(IV-5b)}$$

Equation (IV-4) defines the relationship between Q^+ and c_w^+ for a given combination of N_{Re_x}, b_I^+ and B_2. In order to obtain the numerical results of c_w^+ vs Q^+, a value of Q^+ is specified and the resulting implicit equation in c_w^+ can be solved using Newton Raphson iteration scheme. Comparison between the results of the finite difference solution and those of Equation (IV-4) are given in Figures 13 and 14 for two cases; $b_I^+ = 200$, $N_{Re_x} = 0.006$, $B_2 = 0.5$, and $b_I^+ = 150$, $N_{Re_x} = 0.015$ and $B_2 = 0.5$. In terms of excess salt buildup (i.e. $c_w^+ - 1$), the one-dimensional model yields much lower values and tends to underestimate the extent of concentration polarization. Furthermore, this underestimation increases as one proceeds downstream.

A conventional way of describing the mass transfer characteristic is in terms of the mass transfer coefficient which can be defined as follows:

$$k_x = -\frac{D_s \left(\frac{\partial c}{\partial y}\right)_{y=0}}{c_w - c_b} \qquad \text{(IV-6)}$$

Accordingly, the Sherwood number, N_{Sh}, becomes

$$N_{Sh} = \frac{k_x D_e}{b} = -\left(\frac{\partial c^+}{\partial y^+}\right)_{y^+=0} / (c_w^+ - c_b^+) \qquad \text{(IV-7)}$$

Substituting Equations (II-7) and (IV-3) into Equation (IV-7), one has,

$$N_{Sh} = \frac{k D_n}{b} = \frac{\left[N_{Re_v}\right]\left[N_{Sc}\right](v_w^+)(c_w^+)(1-Q^+)}{(1-Q^+)\,c_w^+ - 1} \qquad \text{(IV-8)}$$

Numerical values of the local Sherwood number as a function of x^+ are shown in Figures 15a and 15b for a variety of cases. For small longitudinal distances ($x^+ \leq 15$), N_{Sh} was found to be essentially independent of B_2. For $x^+ > 20$, N_{Sh} decreases with the increase of B_2. However, the effect to B_2 on N_{Sh} is much less as compared with that on other pertinent parameters (for example, compare Figure 3 with Figure 15).

For a numerical treatment such as given in this work, the question of predicting the results for conditions not specifically covered in the numerical calculation always presents some difficulty because of the absence of the closed-form expression. Owing to the large number parameters involved in this work (i.e., N_{Re_w}, b_I^+, B_2 and N_{Sc}), only limited cases can be considered. The prediction of all pertinent quantities by direct interpolation, therefore, becomes difficult. On the other hand, the most important quantity from a practical point of view is that of the wall concentration, c_w^+. It is believed that a reasonable procedure for the prediction of c_w^+ is through the use of expression for N_{Sh} given by Equation (IV-8). Combining this expression with Equations (II-10) and (II-12) yields,

$$N_{Sh} = \frac{\left[N_{Re_w}\right]\left[N_{Sc}\right]}{(1-B_2)}\, c_w^+ (1-B_2\, c_w^+)\, \frac{(1-B_2) - N_{Re_w} \int_0^{x^+} (1-B_2\, c_w^+)\, dx^+}{(1-B_2)(c_w^+-1) - c_w^+ \left[N_{Re_w}\right] \int_0^{x^+} (1-B_2\, c_w^+)\, dx^+}$$

For a given set of parameters, the local Sherwood number as a function of x^+ can be estimated by interpolation based on the data given in Figures 15a,b. Once this information becomes available, the relationship of c_w^+ vs x^+ can be obtained

from Equation (IV-9). The main advantage of this procedure lies in the fact of the less dependency of N_{Sh} on the parameters, b_Y^+, N_{Re_E} and B_2 as discussed previously. Consequently, one can predict values of N_{Sh} by interpolation with more ease. It should also be noted that in the present work, the Schmidt number is taken as 560 (i.e. NaCl-H_2O System). However, if the well-established relationship of N_{Sh} being proportional to the cubic root of N_{Sc} is assumed to be also valid for the present problem, the performance of a reverse osmosis system in turbulent flow with systems other than NaCl-H_2O can be easily predicted by this procedure.

ACKNOWLEDGEMENT

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NOMENCLATURE

A	= membrane constant
B_2	= $(P_{os})_I/\Delta P$
b	= half the distance between membranes
b^+	= $\frac{b}{\nu}\sqrt{\frac{\tau_w}{\rho}}$
b_I^+	= value of b^+ at inlet
c_B	= bulk concentration
c_B^+	= c_B/c_I
c_I	= salt concentration at inlet
c	= salt concentration
c^+	= c/c_I
c_w	= wall concentration
c_w^+	= c_w/c_I
D	= salt diffusion coefficient
f	= friction factor
G	= defined by Equation (XIV-8)
H	= defined by Equation (XII-9)
i	= position index (x^+ direction)
j	= position index (z^+ direction)
k_x	= defined by Equation (XV-6)
N_{Re}	= bu_E/ν
N_{Re_E}	= $4\,N_{Re}$, Reynolds number based on equivalent diameter
N_{Re_I}	= N_{Re} at inlet = bU_o/ν

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$\left[N_{Re_R}\right]_I$ = N_{Re_R} at inlet

N_{Re_v} = defined as $\frac{bv_{v_o}}{\nu}$

N_{Sc} = Schmidt number, $\frac{\nu}{D}$

P_{os} = osmotic pressure

$(P_{os})_I$ = osmotic pressure at inlet

Q^+ = fraction of water withdrawn

u = axial component of velocity

u^+ = $u/\sqrt{\frac{\tau_w}{\rho}}$

u_1^+ = u^+ at $y^+ = 26$

v_B = bulk velocity

v_{B_o} = bulk velocity at inlet

v = transverse velocity

v^+ = v/v_{v_o}

v_w = wall velocity

v_{v_o} = wall velocity at $x^+ = 0$

x = axial coordinate

x^+ = $x/(b)\ (N_{Re_I})$

y = transverse coordinate

y^+ = $\frac{y}{\nu}\sqrt{\frac{\tau_w}{\rho}}$

z^+ = $y^+/b^+ = y/b$

α = $\frac{1}{1-B_2}$

β = αB_2

Γ = defined by Equation (I-1)

ΔP = pressure drop across the membrane

$\Delta x^+, \Delta z^+$ = increments in x^+ and z^+ directions

ϵ = eddy diffusivity

ϵ^o = weighting factor (= 0.5)

Λ = $\frac{1}{N_{Sc}} + \frac{\varepsilon}{\nu}$

ν = kinematic viscosity

ρ = density

τ_w = wall shear stress

REFERENCES

1. Brian, P.L.T., Ind. Eng. Chem. Fundamentals, 4, 439 (1965).

2. Bruce, G.H., Peaceman, D.W., and Rachford, Jr., Petroleum Transactions A.I.M.E. 198, 79 (1953).

3. Deissler, R.G., NACA TN 3145 (1954).

4. Dresner, L., Oak Ridge National Laboratory Report No. ORNL 3621 (May 1964).

5. Gill, W.N., Tien, Chi, and Zeh, D.W., Ind. Eng. Chem. Fundamentals 4, 433 (1965).

6. Gill, W.N., Tien, Chi, and Zeh, D.W., Int. J. Heat and Mass Transfer 9, 907 (1966).

7. Merten, U., Lonsdale, H.K., and Riley, R.L., Ind. Eng. Chem. Fundamentals, 3, 210 (1964).

8. Sherwood, T.K., Brian, P.L.T., Fisher, R.E., M.I.T. Report No. 295-1 OSR 9336 (1963).

9. Sherwood, T.K., Brian, P.L.T., Fisher, R.E., and Dresner, L., Ind. Eng. Chem. Fundamentals 4, 113 (1965).

10. Srinivasan, S., Tien, Chi., and Gill, W.N., Chem. Eng. Sci. 22, 417 (1967).

11. Srinivasan, S., and Tien, Chi., "Reverse Osmosis Desalination in Tubular Membrane Duct", presented before the Second European Symposium on Fresh Water from the Sea, May 9-12 (1967) Athens, Greece, to be published in Desalination.

TABLE I

$N_{Re_w} = 0.006 \quad B_2 = 0.25$

x^+ Based on $b_I^+ = 300$	$b_I^+ = 300$ $\left[N_{Re_E}\right]_I = 20941$		$b_I^+ = 200$ $\left[N_{Re_E}\right]_I = 13175$		$b_I^+ = 150$ $\left[N_{Re_E}\right]_I = 9484$		$b_I^+ = 100$ $\left[N_{Re_E}\right]_I = 5967$	
	Q^+	$\left[N_{Re_E}\right]_I (Q^+)$	Q^+	$\left[N_{Re_E}\right]_I (Q^+)$	Q^+	$\left[N_{Re_E}\right]_I (Q^+)$	Q^+	$\left[N_{Re_E}\right]_I (Q^+)$
1.0	0.005927	124.12	0.00934	123.0	0.01294	122.72	0.02022	120.65
5.0	0.0294	615.24	0.0467	612.24	0.0641	607.50	0.0991	591.38
10.0	0.05826	1220	0.09174	1209	0.1246	1187	0.191	1139
15.0	0.087	1822	0.1353	1782	0.1847	1752	0.2734	1631
20.0	0.1147	2402	0.1786	2353	0.2406	2282	0.3487	2081

TABLE II

$N_{Re_V} = 0.015 \quad B_2 = 0.5$

x^+ Based on $b_I^+ = 300$	$b_I^+ = 300$ $\left[N_{Re_E}\right]_I = 20941$		$b_I^+ = 200$ $\left[N_{Re_E}\right]_I = 13175$		$b_I^+ = 150$ $\left[N_{Re_E}\right]_I = 9484$		$b_I^+ = 100$ $\left[N_{Re_E}\right]_I = 5967$	
	Q^+	$\left[N_{Re_E}\right]_I (Q^+)$	Q^+	$\left[N_{Re_E}\right]_I (Q^+)$	Q^+	$\left[N_{Re_E}\right]_I (Q^+)$	Q^+	$\left[N_{Re_E}\right]_I (Q^+)$
1.0	0.01397	292.54	0.02139	261.76	0.0286	271.63	0.04174	249.0
5.0	0.06676	1398	0.09986	1316	0.1278	1212	0.1717	1024
10.0	0.1259	2637	0.1804	2377	0.2198	2084	0.2652	1582
15.0	0.1783	3733	0.2423	3192	0.2830	2684	0.3105	1852
20.0	0.2221	4650	0.2899	3819	0.3209	3043	0.332	1981

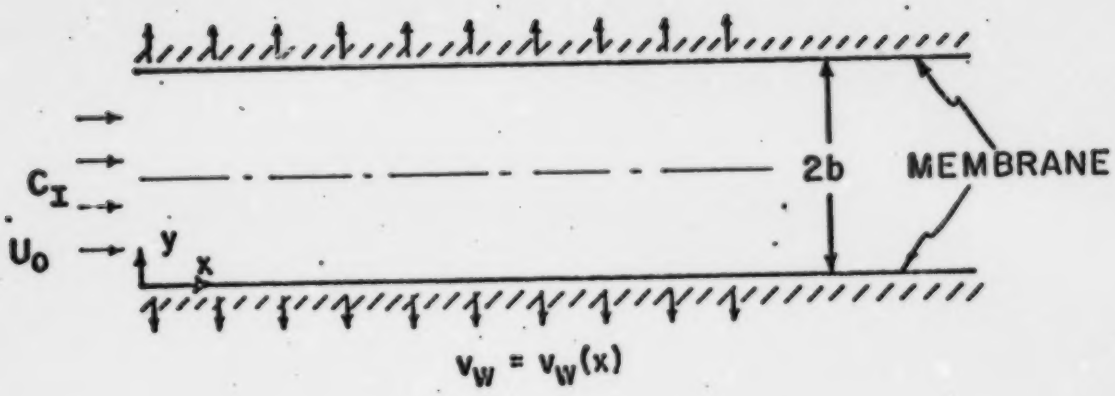

FIG. 1 SCHEMATIC DIAGRAM OF REVERSE OSMOSIS DUCT.

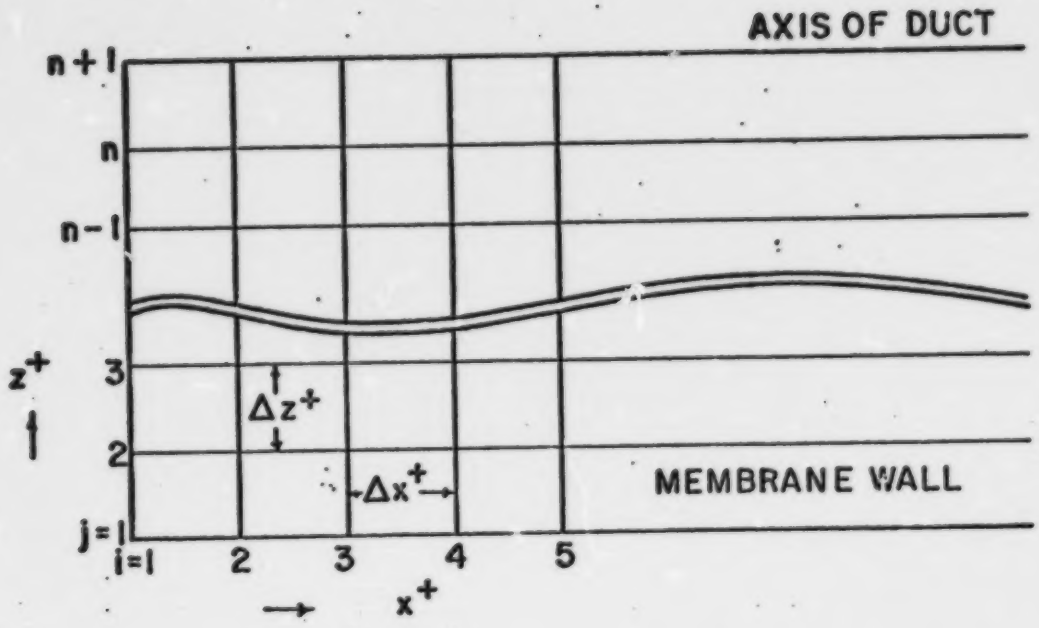

FIG. 2 MESH NET WORK.

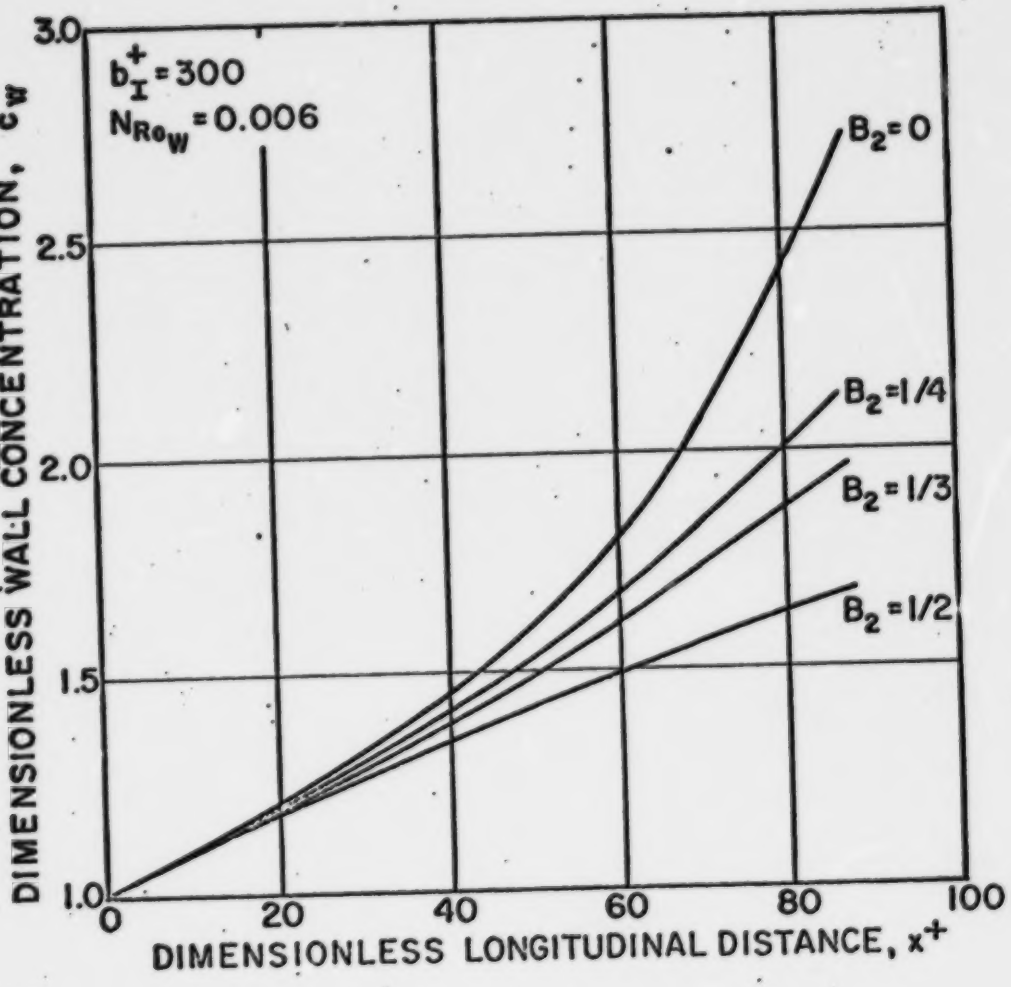

FIG. 3 DIMENSIONLESS CONCENTRATION AS A FUNCTION OF DIMENSIONLESS LONGITUDINAL DISTANCE.

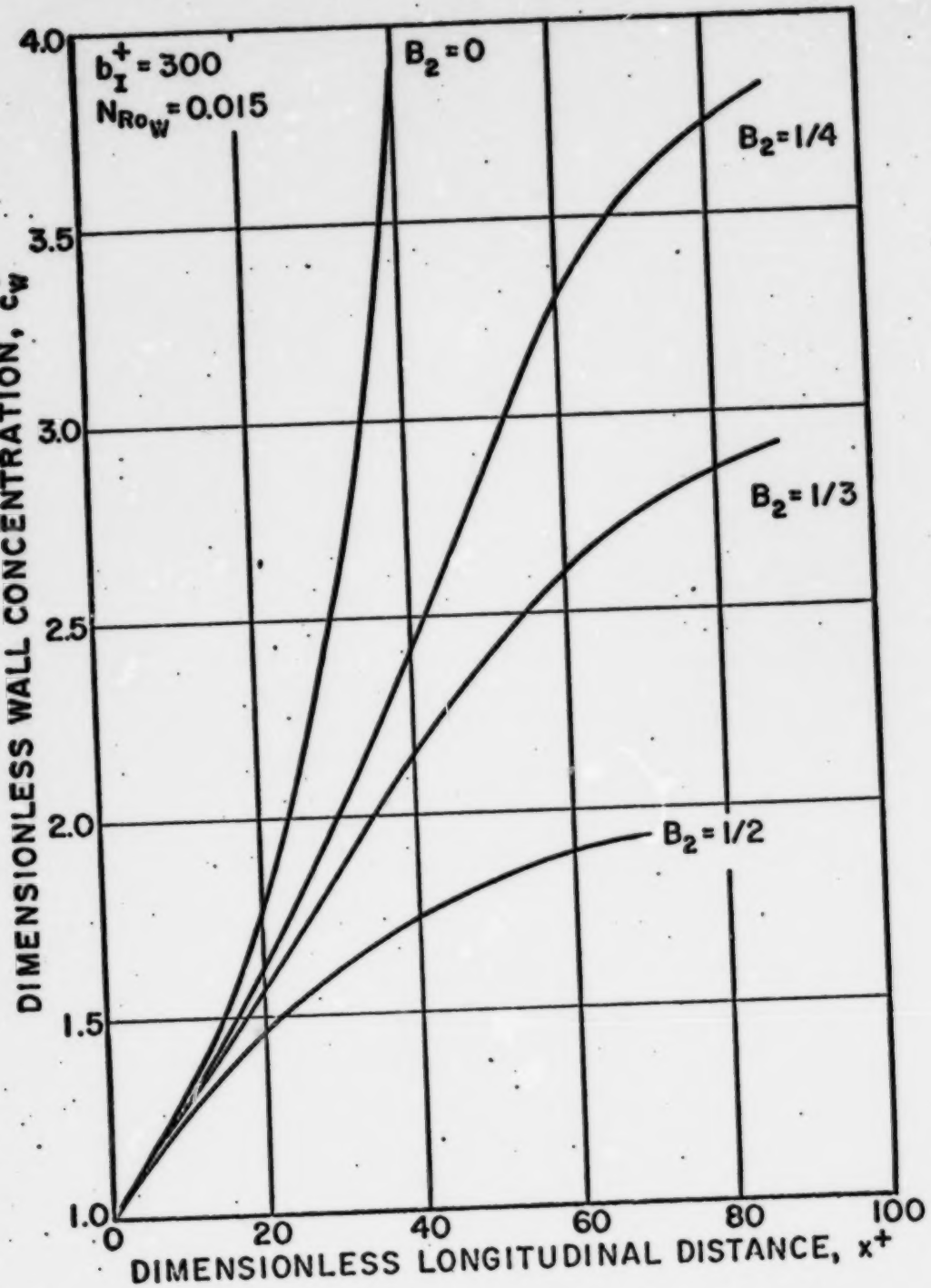

FIG. 4 DIMENSIONLESS CONCENTRATION AS A FUNCTION OF DIMENSIONLESS LONGITUDINAL DISTANCE.

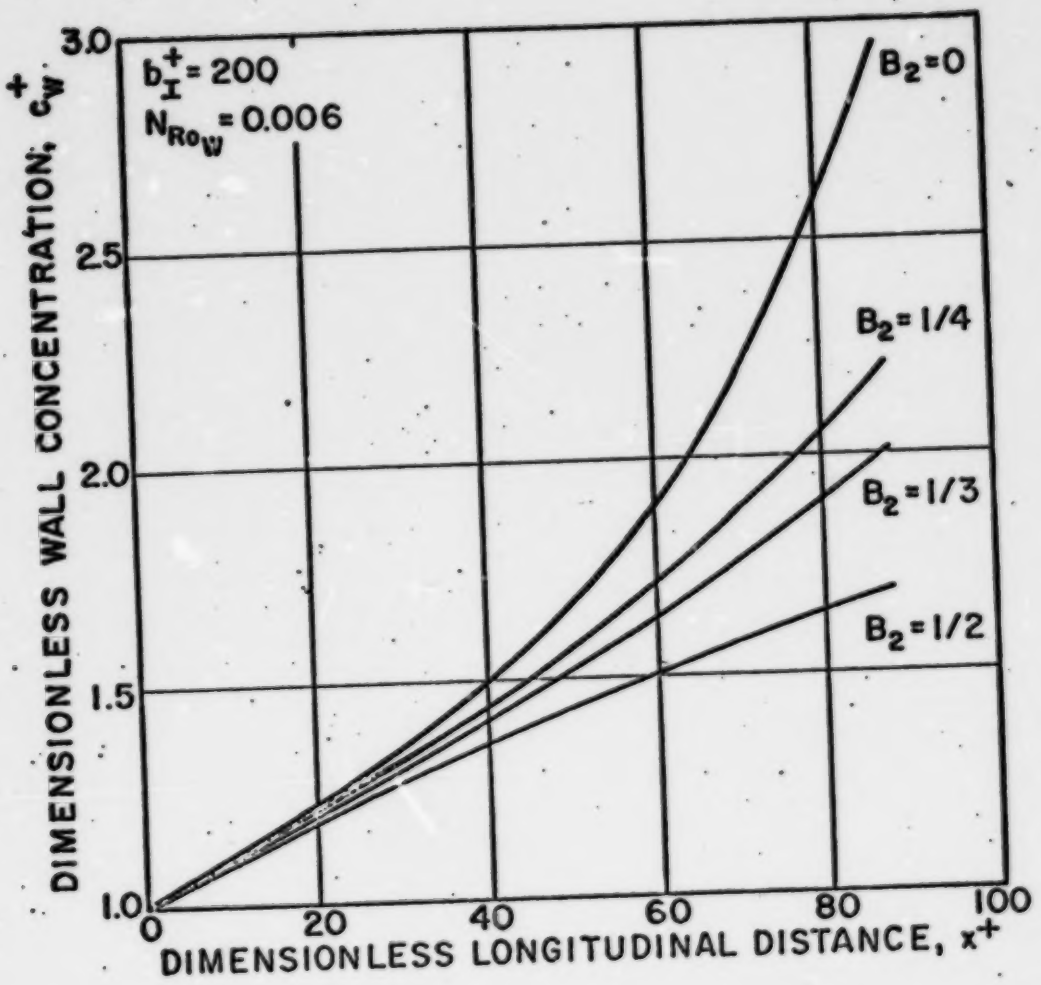

FIG. 5 DIMENSIONLESS CONCENTRATION AS A FUNCTION OF DIMENSIONLESS LONGITUDINAL DISTANCE.

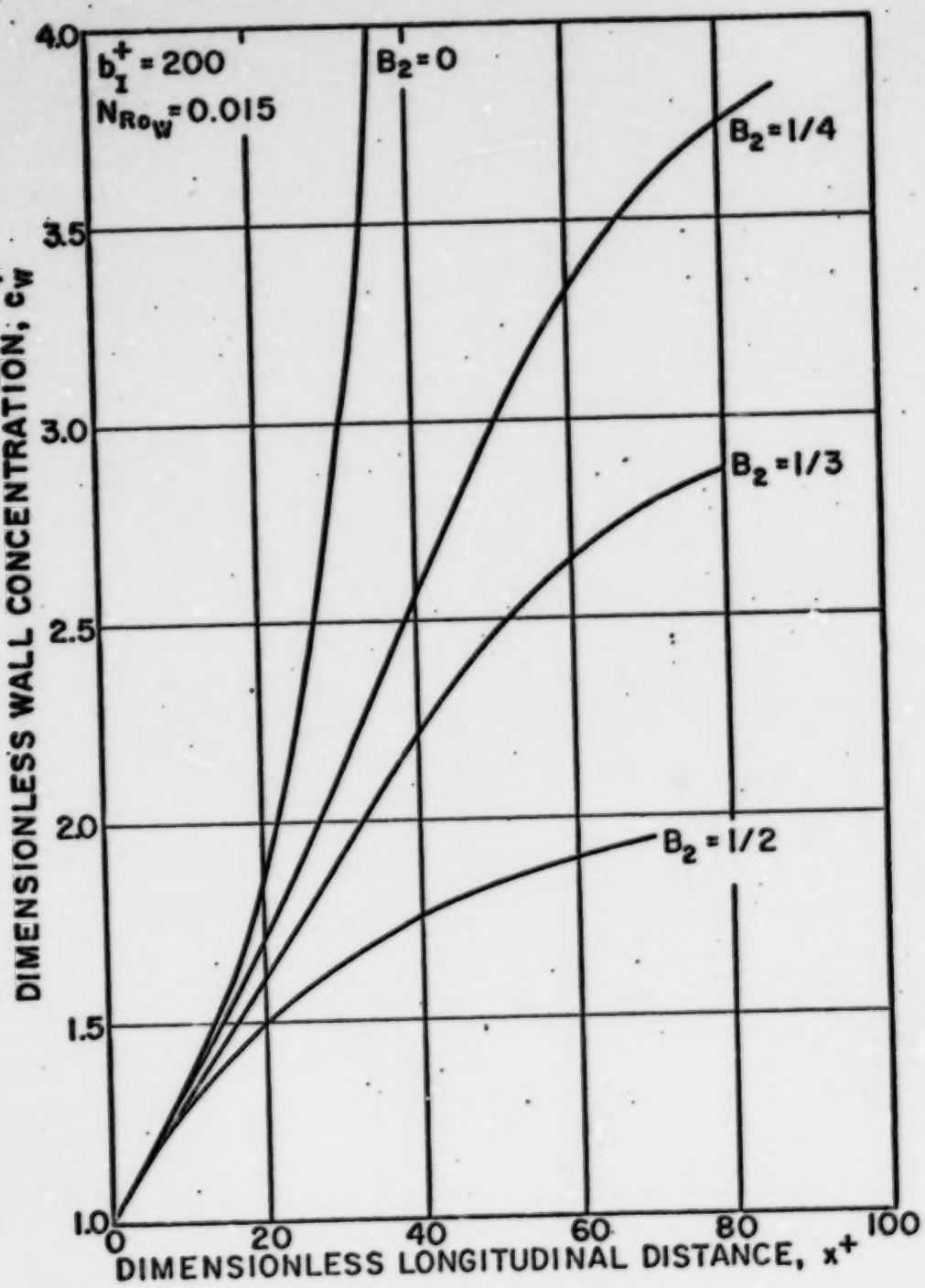

FIG. 6 DIMENSIONLESS CONCENTRATION AS A FUNCTION OF DIMENSIONLESS LONGITUDINAL DISTANCE.

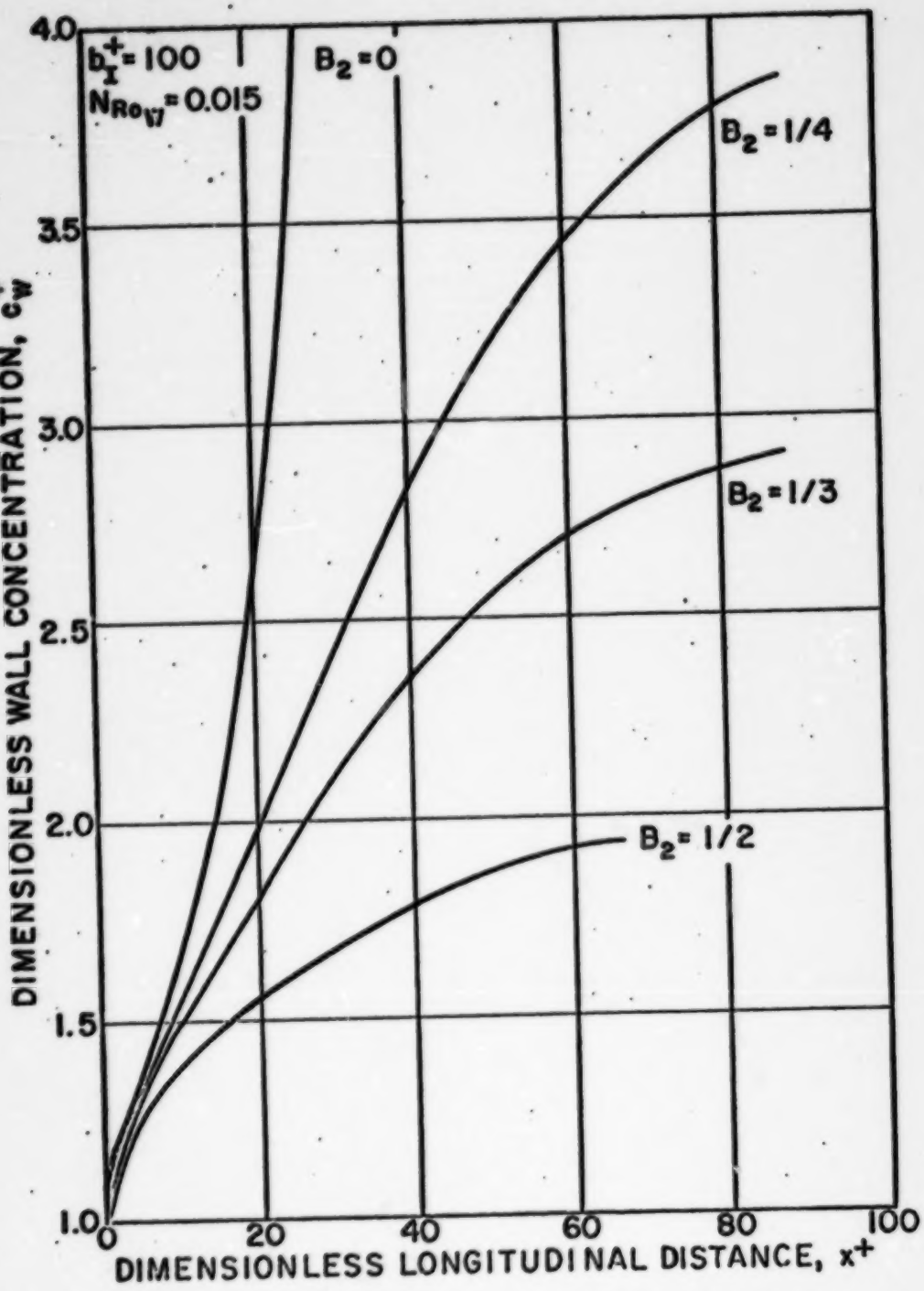

FIG. 7 DIMENSIONLESS CONCENTRATION AS A FUNCTION OF DIMENSIONLESS LONGITUDINAL DISTANCE.

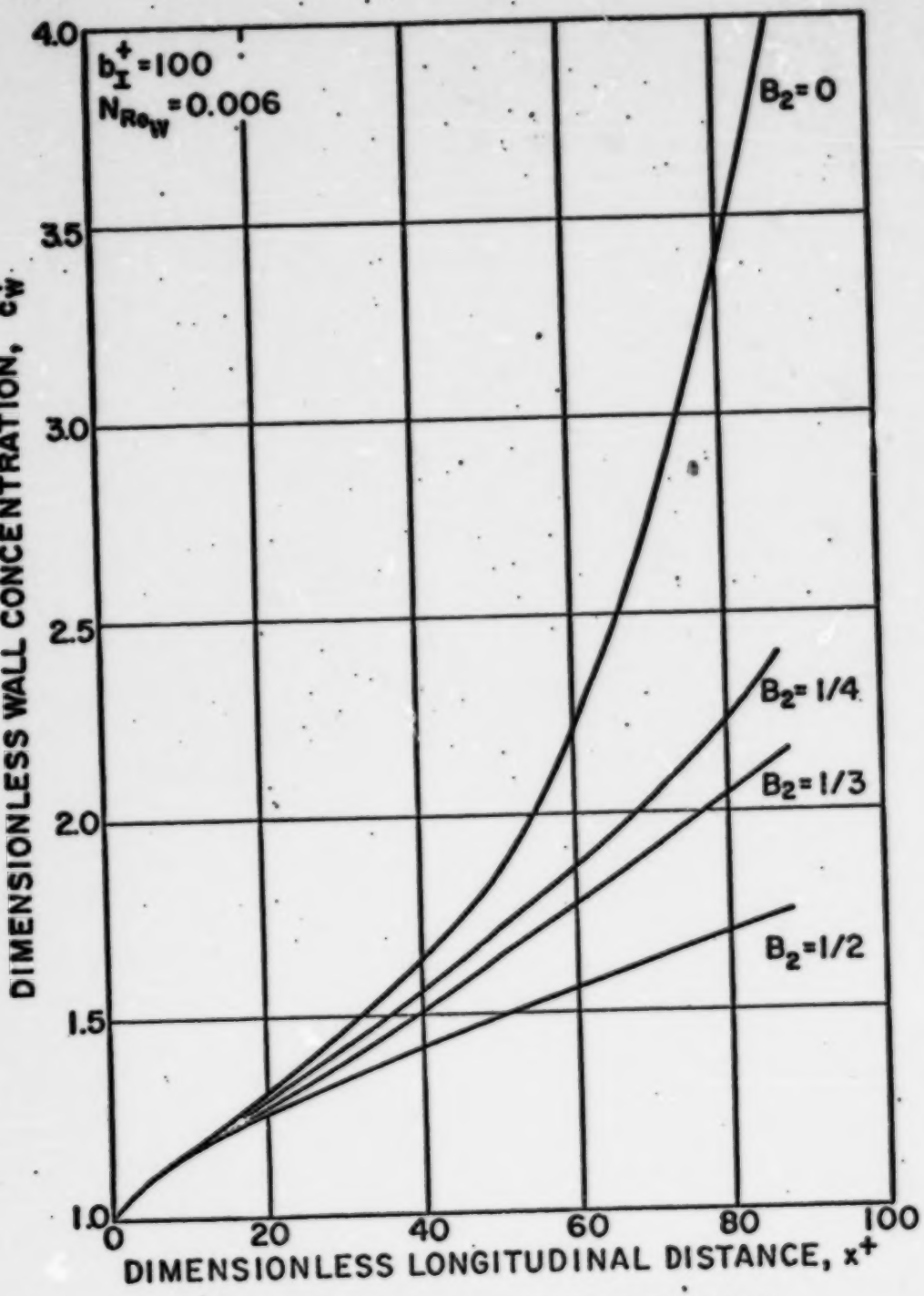

FIG. 8 DIMENSIONLESS CONCENTRATION AS A FUNCTION OF DIMENSIONLESS LONGITUDINAL DISTANCE.

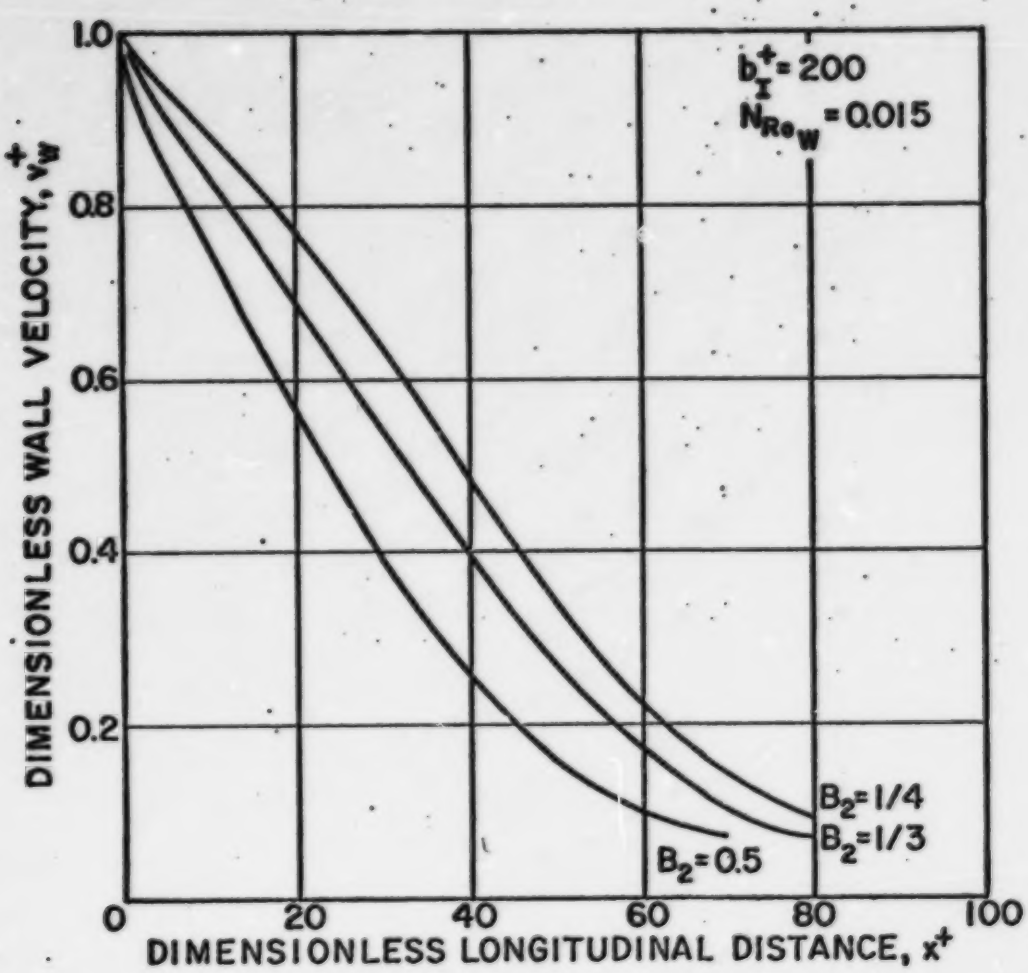

FIG. 9 DIMENSIONLESS WALL VELOCITY VS. DIMENSIONLESS AXIAL DISTANCE.

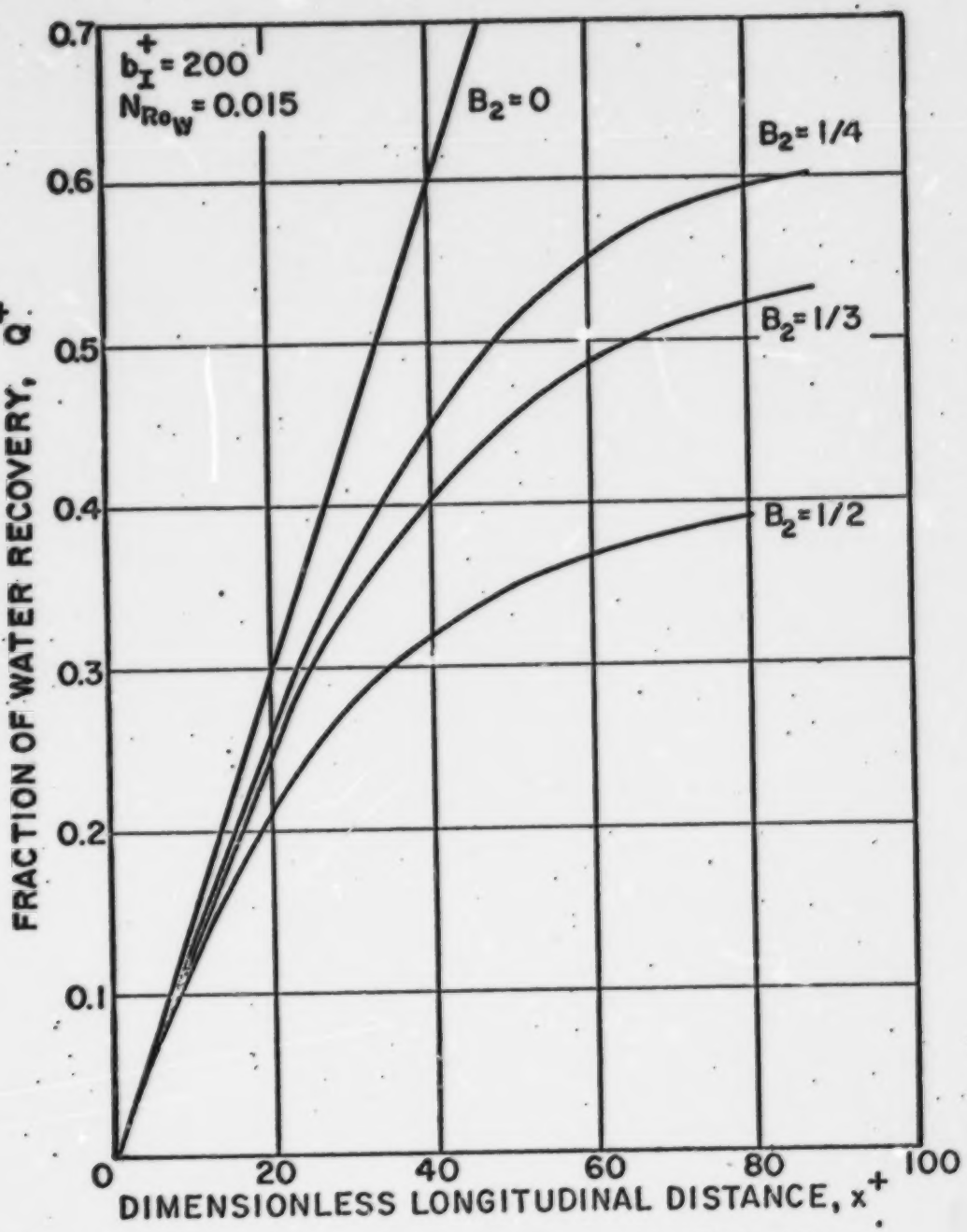

FIG. 10 FRACTION OF WATER RECOVERY VS. DIMENSIONLESS LONGITUDINAL DISTANCE.

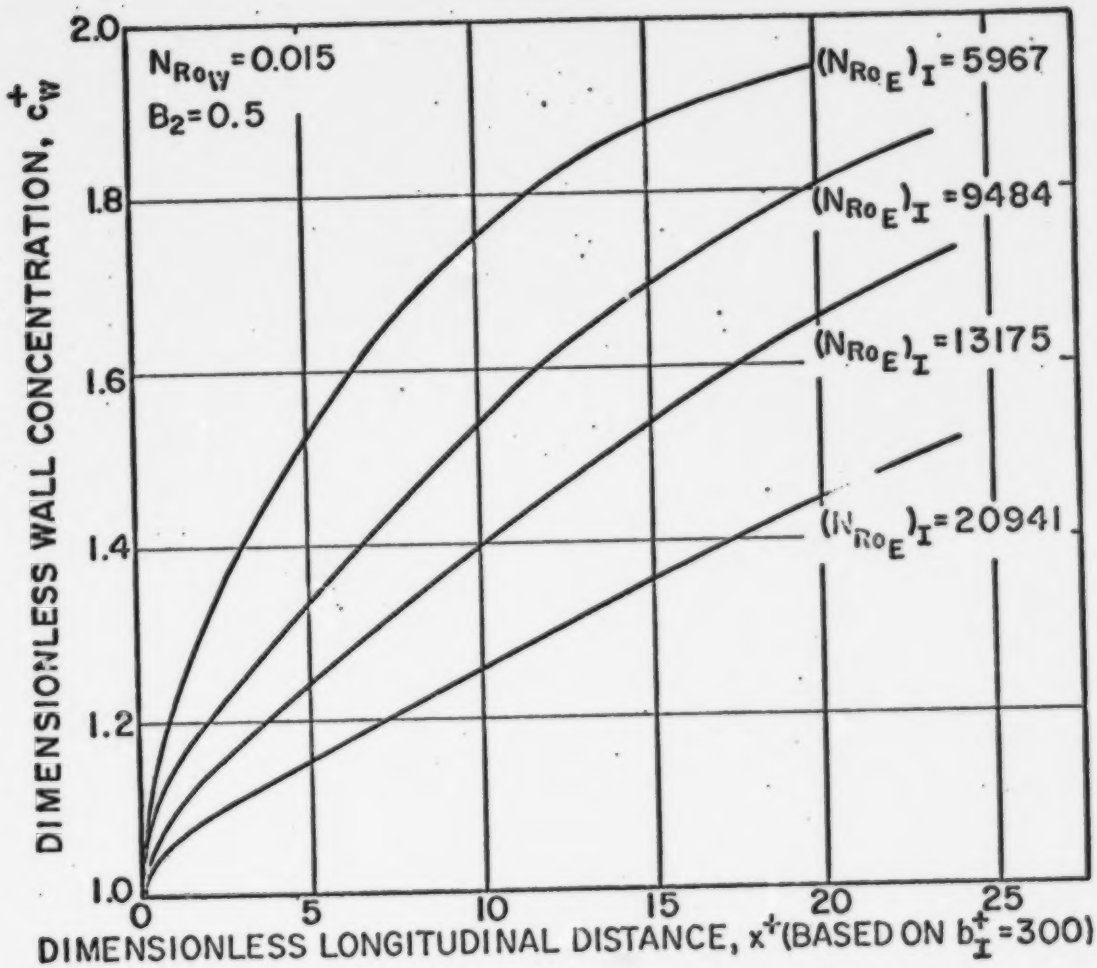

FIG. 11 EFFECT OF INLET REYNOLDS NUMBER ON CONCENTRATION POLARIZATION.

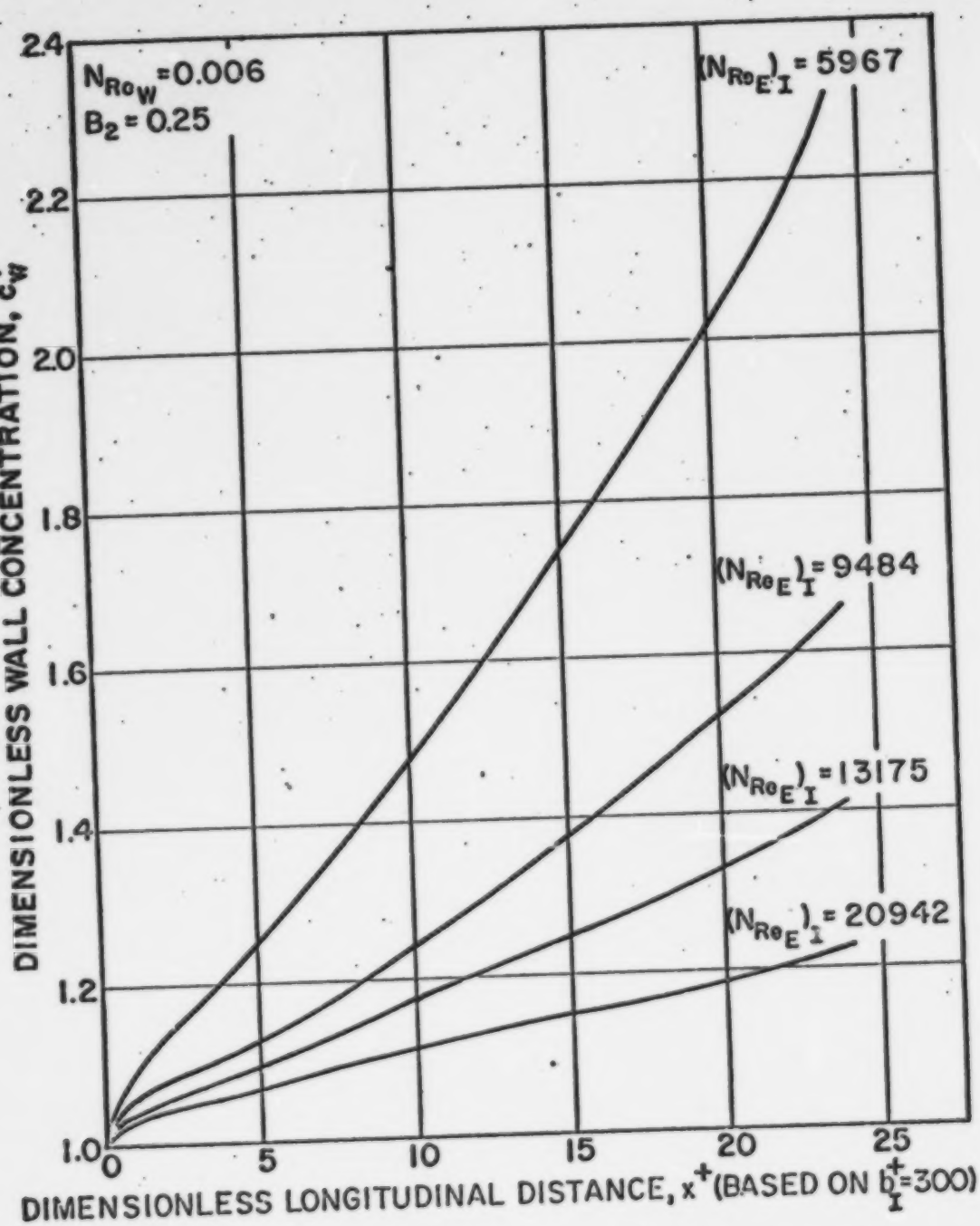

FIG. 12 EFFECT OF INLET REYNOLDS NUMBER ON CONCENTRATION POLARIZATION.

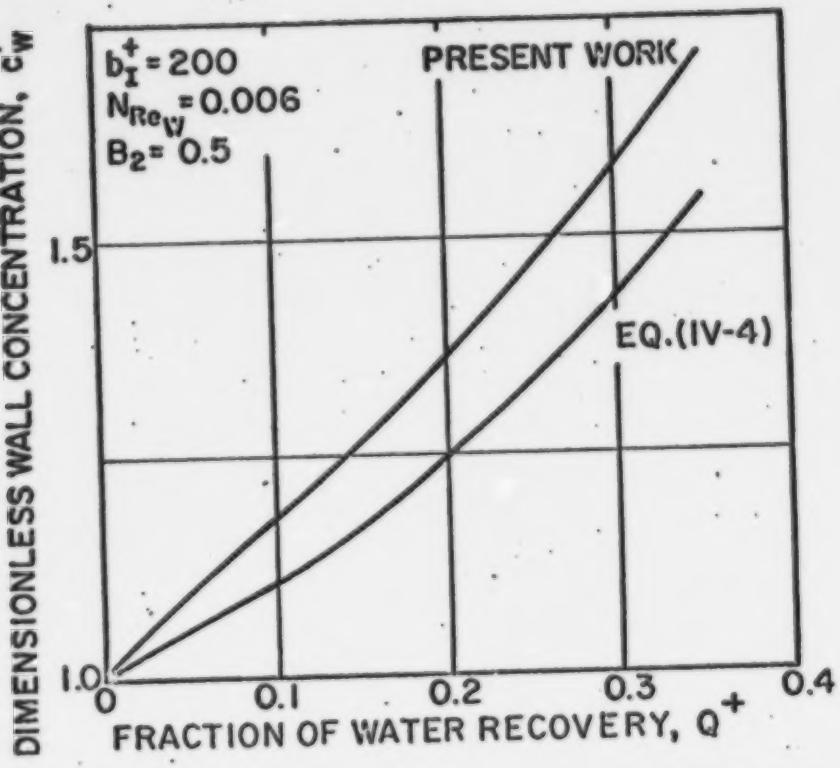

FIG. 13 COMPARISON BETWEEN PRESENT INVESTIGATION AND THAT BASED ON ONE DIMENSIONAL DIFFUSION MODEL.

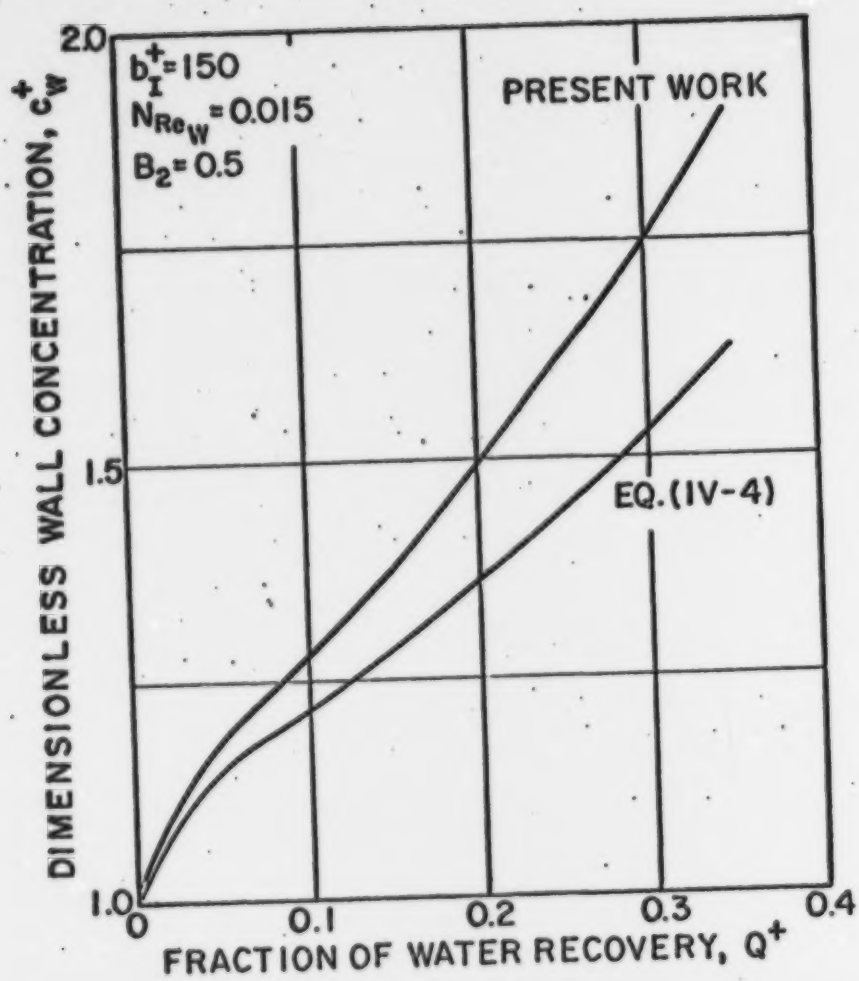

FIG. 14 COMPARISON BETWEEN PRESENT INVESTIGATION AND THAT BASED ON ONE DIMENSIONAL DIFFUSION MODEL.

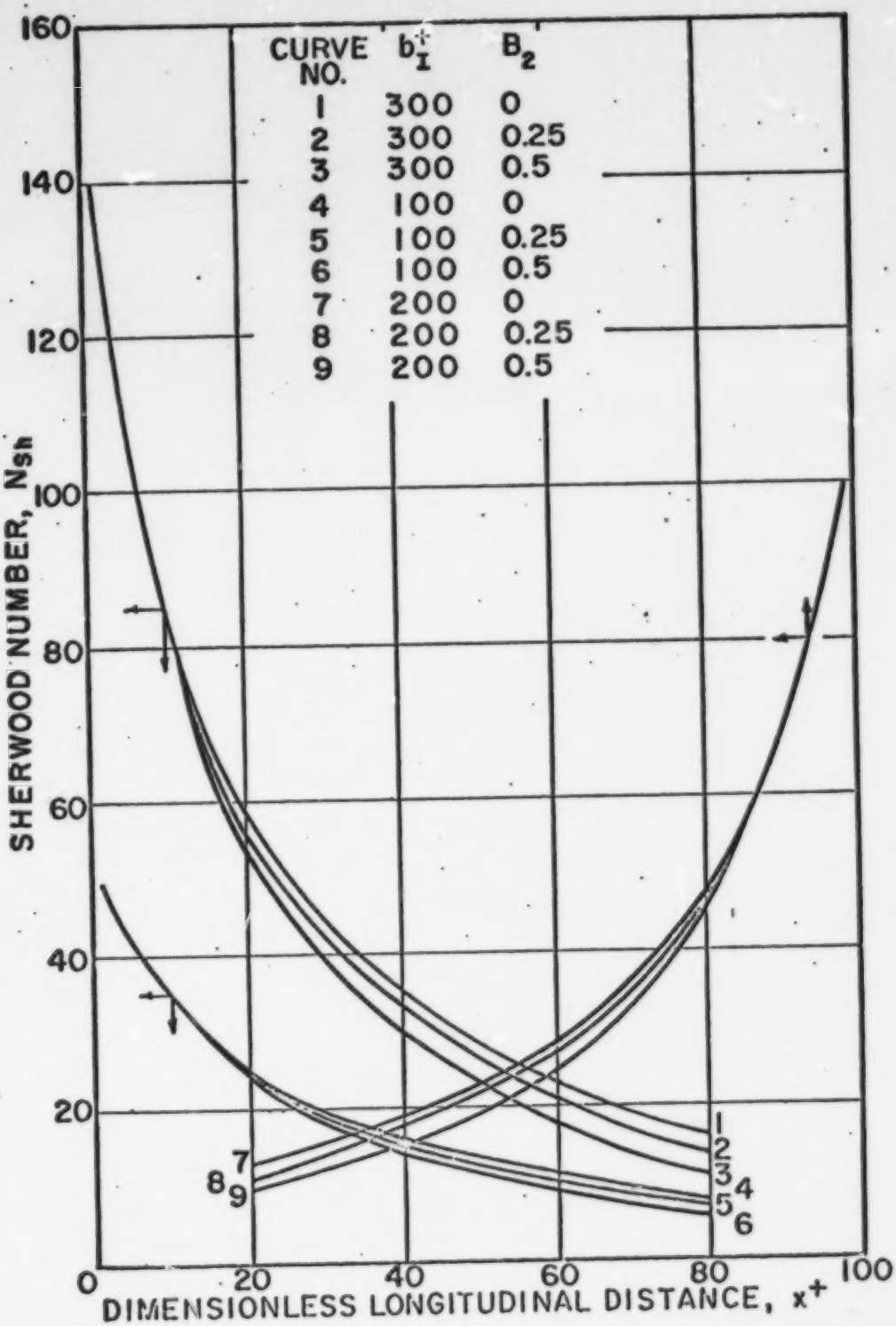

FIG. 15a SHERWOOD NUMBER VS. DIMENSIONLESS LONGITUDINAL DISTANCE.

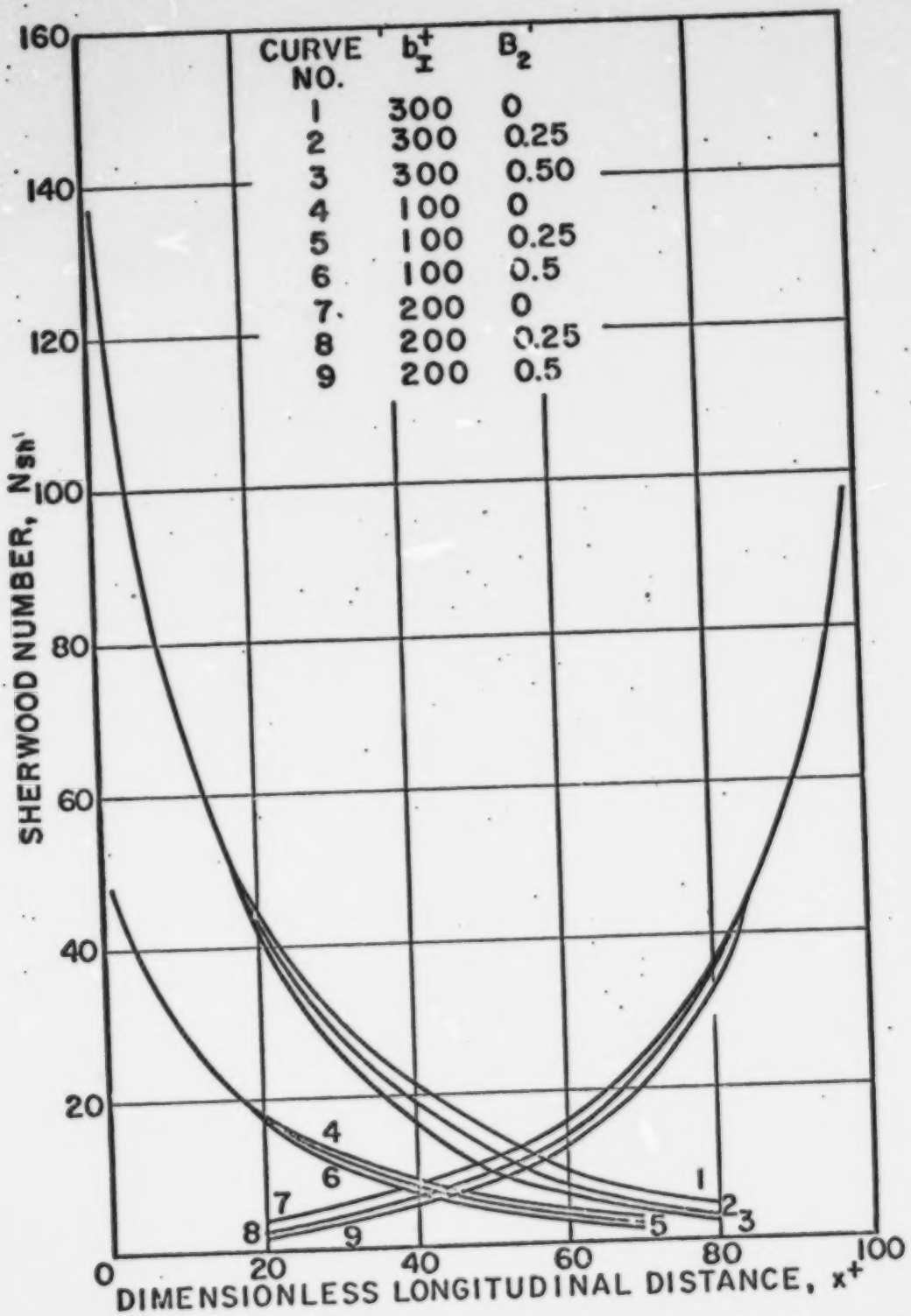

FIG. 15b SHERWOOD NUMBER VS. DIMENSIONLESS LONGITUDINAL DISTANCE.

Reverse Osmosis in Multicomponent Systems

by

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ABSTRACT

A mathematical analysis based on boundary layer theory is presented for the case of reverse osmosis in multicomponent systems. The integral method is used to solve the nonlinear convective diffusion problem. Typical results are shown for ternary systems. Numerical examples are given to illustrate how one of the solutes could exceed the saturation concentration and precipitate. The analysis assumes flat velocity and concentration profiles at the entrance, two dimensional laminar flow, steady state and constant physical properties. The analysis is applicable to both short- and long-conduit cases.

REVERSE OSMOSIS IN MULTICOMPONENT SYSTEMS

INTRODUCTION

Several theoretical studies concerning the problem of diffusion in reverse osmosis systems have appeared in the literature (1 through 12) for both laminar and turbulent flows and for different geometric configurations. These studies, however, confine themselves to binary systems (a single solute in solution). In practice, it is safe to assume that the liquid systems treated by reverse osmosis would always contain more than one species of solute. In such cases, a realistic analysis should take into account the interaction between the various species of solutes and the results for such analyses would enable the prediction of concentration built up along the membrane surface for each and every solute. This information is particularly useful in determining the possibility of precipitation of certain species of solutes due to over-saturation, which has been a major problem of membrane processes.

Two main effects result in multicomponent reverse osmosis systems. First, owing to cross diffusivities, additional terms appear in the diffusion equations. Secondly, the diffusion equations of the individual components are also coupled through the boundary conditions as well as through the velocity associated with the convective term in the equation of change. This is because the effective osmotic pressure is dependent on the total concentration of the solutes. An exact assessment of the first effect is difficult; however, in most cases the cross term of the diffusion flux is at least one order of magnitude less than that of the main term. Consequently,

the multicomponent diffusion problem will be studied only in terms of the combined effect of the species on the effective osmotic pressure.

In the following section, a boundary layer analysis of the mass transfer characteristics of a ternary system in reverse osmosis operation is presented. The approximate integral method is used for the solution of the pertinent equations. This method is used because of its previous success in studying mass transfer problems in reverse osmosis. Although the analysis is given for a ternary system, the approach can easily be generalized to liquid systems with an arbitrary number of species of solutes.

MATHEMATICAL ANALYSIS

The schematic description of the problem is given in Figure 1. The feed solution containing two species of solutes is flowing through a flat duct which consists of two parallel flat membranes, placed at a distance of 2b. If the usual boundary layer assumptions are assumed to be valid, the pertinent equations are written as:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{1}$$

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \overline{U} \frac{d\overline{U}}{dx} + \nu \frac{\partial^2 u}{\partial y^2} \tag{2}$$

$$u \frac{\partial C_1}{\partial x} + v \frac{\partial C_1}{\partial y} = D_{11} \frac{\partial^2 C_1}{\partial y^2} + D_{12} \frac{\partial^2 C_2}{\partial y^2} \tag{3}$$

$$u \frac{\partial C_2}{\partial x} + v \frac{\partial C_2}{\partial y} = D_{21} \frac{\partial^2 C_1}{\partial y} + D_{22} \frac{\partial^2 C_2}{\partial y^2} \tag{4}$$

The subscripts 1 and 2 refer to the first and second solutes, respectively.

The boundary conditions are:

$$u = o, \qquad v = -V_w \qquad \text{at } y = o \tag{5}$$

$$-D_{11}\frac{\partial C_1}{\partial y} - D_{12}\frac{\partial C_2}{\partial y} = V_w C_1 \qquad \text{at } y = o \tag{6}$$

$$-D_{21}\frac{\partial C_1}{\partial y} - D_{22}\frac{\partial C_2}{\partial y} = V_w C_2 \qquad \text{at } y = o \tag{7}$$

Equations (6) and (7) imply the condition of complete salt rejection at the membrane surface.

The permeation velocity across the membrane wall, V_w, is assumed to be given by the phenomenological relationship:

$$V_w = A(\Delta P - P_{os}) \tag{8}$$

where ΔP is the pressure difference across the membrane and P_{os} is the osmotic pressure corresponding to the concentrations at the membrane surface.

The osmotic pressure, P_{os}, in general, is a function of the concentrations of both species. As an approximation, P_{os} is assumed to be a linear function of the total concentration. V_w becomes:

$$V_w = A\,(\Delta P)\,\left[1 - B_2\,\frac{(C_1)_w + (C_2)_w}{(C_1)_o + (C_2)_o}\right] \tag{9}$$

where

$$B_2 = \frac{(P_{os})_o}{\Delta P} \tag{10}$$

The subscript o refers to the inlet condition. The concentrations, C_1 and C_2, are expressed on an equivalent basis.

Before proceeding with the solution of these equations, certain simplifications need to be made. As stated previously, information on the values D_{12} (or D_{21}) is usually not available. Furthermore, the cross diffusion term is at least one order of magnitude less than the main term; consequently these terms will be neglected. With this simplification, Equations (1) through (4) can be written in the following dimensionless form:

$$\frac{\partial u^+}{\partial x^+} + \frac{\partial v^+}{\partial y^+} = 0 \tag{11}$$

$$u^+ \frac{\partial u^+}{\partial x^+} + v^+ \frac{\partial u^+}{\partial y^+} = \bar{U}^+ + \frac{d\bar{U}^+}{dx^+} + \frac{\partial^2 u^+}{\partial y+2} \tag{12}$$

$$u^+ \frac{\partial C_j^+}{\partial x^+} + v^+ \frac{\partial C_j^+}{\partial y^+} = \frac{1}{(N_{Sc})_j} \frac{\partial^2 C_j}{\partial y+2} \qquad j=1,2 \tag{13}$$

Similarly, the boundary conditions become:

$$u^+ = o, \qquad v^+ = -v_w^+ \qquad \text{at } y^+ = o \tag{14}$$

$$-\frac{\partial C_1}{\partial y^+} = B_1 (C_1^+)_w \left[1 - B_2 \frac{r_{12}(C_1^+)_w + (C_2^+)_w}{r_{12} + 1}\right] \qquad \text{at } y^+ = o \tag{15}$$

$$-\frac{\partial C_2}{\partial y^+} = B_1 \frac{N_{Sc_2}}{N_{Sc_1}} (C_2^+)_w \left[1 - B_2 \frac{r_{12}(C_1^+)_w + (C_2^+)_w}{r_{12} + 1}\right] \qquad \text{at } y^+ = o \tag{16}$$

where

$$B_1 = \frac{A\,(\Delta P)\,b}{D_{11}} \tag{17}$$

and

$$r_{12} = \frac{(C_1)_o}{(C_2)_o} \tag{18}$$

The dimensionless wall velocity is given by

$$V_w^+ = \frac{B_1}{N_{Sc_1}} \left[1 - B_2 \frac{r_{12}(C_1^+)_w + (C_2^+)_w}{r_{12} + 1}\right] \tag{19}$$

The dimensionless boundary layer equation (Equation (12)) is now integrated from $y^+ = 0$ to $y^+ = \delta^+$ where δ^+ is the dimensionless momentum boundary layer thickness. Using the conditions

$$u^+ = 0 \text{ at } y^+ = 0 \tag{20}$$

and

$$u^+ = \overline{U}^+, \quad \frac{\partial u^+}{\partial y^+} = 0 \quad \text{at } y^+ = \delta^+ \tag{21}$$

one gets the following equation:

$$\frac{d}{dx^+} \int_o^{\delta^+} (\overline{U}^+ - u^+)\, u^+\, dy^+ + \frac{d\overline{U}^+}{dx^+} \int_o^{\delta^+} (\overline{U}^+ - u^+)\, dy^+ = \left(\frac{\partial u^+}{\partial y^+}\right)_{y^+=0} - V_w^+ \overline{U}^+ \tag{22}$$

The velocity profile (satisfying Equations (20) and (21)) is assumed to be:

$$\frac{u^+}{\overline{U}^+} = 2\frac{Y^+}{\delta^+} - \left(\frac{Y^+}{\delta^+}\right)^2 \tag{23}$$

A relationship between $\bar{U}^+$, δ^+ and x^+ may be readily obtained by a material balance.

$$U^+ = \frac{3(1 - \int_0^{x^+} V_w^+ \, dx^+)}{3 - \delta^+} \tag{24}$$

Using Equations (23) and (24) in Equation (22), one gets, after some rearrangement,

$$\frac{d\delta^+}{dx^+} = \frac{\frac{2}{\delta^+} + V_w^+ \left(\frac{9}{5} \frac{\delta^+}{3-\delta^+} - 1\right)}{\left(\frac{1 - \int_0^{x^+} V_w^+ \, dx^+}{3 - \delta^+}\right)\left(\frac{2}{5} + \frac{9}{5} \frac{\delta^+}{3-\delta^+}\right)} \tag{25}$$

The integral equation for the concentration field may now be obtained. There are two dimensionless concentration boundary layers, and their thicknesses (dimensionless) are designated as Δ_1^+ and Δ_2^+, respectively. By integrating Equation (13) from $y^+ = 0$ to $y^+ = \Delta_j^+$ (j=1,2), one gets:

$$\frac{d}{dx^+} \int_0^{\Delta_j^+} u^+ (1-C_j^+) \, dy^+ + V_w^+ [1-(C_j^+)_w] = \frac{1}{(N_{Sc})_j} \left(\frac{\partial C_j^+}{\partial y^+}\right)_{y^+=0} \tag{26}$$

The boundary layer assumption requires that

$$C_j^+ = 1, \qquad \frac{\partial C_j^+}{\partial y^+} = 0 \quad \text{at } y^+ = \Delta_j^+ \tag{27}$$

The concentration profiles are assumed to be as follows:

$$C_1^+ = a_1 + a_2 \frac{y^+}{\Delta_1^+} + a_3 \frac{y^{+2}}{\Delta^{+2}} \tag{28}$$

$$C_2^+ = b_1 + b_2 \frac{y^+}{\Delta_2^+} + b_3 \frac{y^{+2}}{\Delta_2^{+2}} \tag{29}$$

The coefficients a_i, b_i (i=1,2,3) may be determined from compatibility requirements. From Equations (27)-(29), one has:

$$a_1 + a_2 + a_3 = 1 \tag{30}$$

$$b_1 + b_2 + b_3 = 1 \tag{31}$$

$$a_2 + 2a_3 = 0 \tag{32}$$

$$b_2 + 2b_3 = 0 \tag{33}$$

Also with these concentration profiles, Equations (15) and (16) become:

$$-\frac{a_2}{\Delta_1^+} = B_1 a_1 \left[1 - B_2 \frac{r_{12} a_1 + b_1}{r_{12} + 1}\right] \tag{34}$$

$$-\frac{2(1-b_1)}{\Delta_2^+} = B_1 \frac{(N_{Sc})_2}{(N_{Sc})_1} b_1 \left[1 - B_2 \frac{r_{12} a_1 + b_1}{r_{12} + 1}\right] \tag{35}$$

From Equations (30)-(33) one gets:

$$a_2 = 2(1-a_1) \tag{36}$$

$$b_2 = 2(1-b_1) \tag{37}$$

$$a_3 = a_1 - 1 \tag{38}$$

$$b_3 = b_1 - 1 \tag{39}$$

Thus, Equations (34) and (35) give explicit expressions for Δ_1^+ and Δ_2^+ in terms of a_1, b_1 and the system parameters.

Substituting the velocity and concentration profiles into Equation (26) and after some rearrangements, the following equations are obtained:

$$\frac{d}{dx^+}\left[\bar{U}^+ (1 - a_1) \frac{\Delta_1^{+2}}{\delta^+}\right] = \frac{12}{(N_{Sc})_1} \frac{1-a_1}{\Delta_1^+} - 6 V_w^+ (1 - a_1) \tag{40}$$

$$\frac{d}{dx^+}\left[\bar{U}^+ (1 - b_1) \frac{\Delta_2^{+2}}{\delta^+}\right] = \frac{12}{(N_{Sc})_2} \frac{1-b_1}{\Delta_2^+} - 6 V_w^+ (1 - b_1) \tag{41}$$

One can eliminate the quantities of Δ_1^+ and Δ_2^+ of Equations (40) and (41) through the use of Equations (34) and (35). After carrying out the differentiations in Equations (40) and (41) and with some rearrangement, the following system of equations results:

$$f_1 \frac{da_1}{dx^+} + f_2 \frac{db_1}{dx^+} = f_3 \tag{42}$$

$$g_1 \frac{da_1}{dx^+} + g_2 \frac{db_1}{dx^+} = g_3 \tag{43}$$

where

$$f_1 = \bar{U}^+ \frac{\Delta_1^+}{\delta^+} [2(1-a_1) p_1 - \Delta_1^+] \tag{44}$$

$$f_2 = \frac{2 \bar{U}^+ (1-a_1) \Delta_1^+}{\delta^+} p_2 \tag{45}$$

$$f_3 = (1-a_1)\left[\frac{12}{(N_{Sc})_1}\frac{1}{\Delta_1^+} - 6\,V_w^+ + \frac{\bar{U}^+\Delta_1^{+2}}{\delta^{+2}}\frac{d\delta^+}{dx^+} - \frac{\Delta_1^{+2}}{\delta^+}\frac{d\bar{U}^+}{dx^+}\right] \tag{46}$$

$$p_1 = \frac{2a_1\,V_w^+\,(N_{Sc})_1 + 2B_1(1-a_1)\left[1 - \frac{B_2}{r_{12}+1}(2r_{12}\,a_1 + b_1)\right]}{a_1^{\,2}\,(V_w^+)\,(N_{Sc})_1^{\,2}} \tag{47}$$

$$p_2 = \frac{2B_1B_2\,(a_1 - 1)}{(r_{12}+1)a_1\,(V_w^+)^2\,(N_{Sc_1})^2} \tag{48}$$

$$g_1 = \frac{\bar{U}^+\Delta_2^+}{\delta^+}\,[2(1-b_1)\,q_1] \tag{49}$$

$$g_2 = \frac{\bar{U}^+\Delta_2^+}{\delta^+}\,[\,2(1-b_1)\,q_1 - \Delta_2^+\,] \tag{50}$$

$$g_3 = (1-b_1)\left[\frac{12}{(N_{Sc})_2}\,\frac{1}{\Delta_2^+} - 6\,V_w^+ + \frac{\bar{U}^+\Delta_2^{+2}}{\delta^{+2}}\frac{d\delta^+}{dx^+} - \frac{\Delta_2^{+2}}{\delta^+}\frac{d\bar{U}^+}{dx^+}\right] \tag{51}$$

$$q_1 = \frac{2(b_1-1)\,r_{12}\,B_1\,B_2}{(r_{12}+1)(N_{Sc})_1(N_{Sc})_2(V_w^+)^2\,b_1} \tag{52}$$

$$q_2 = \frac{2b_1\,V_w^+ + \frac{2B_1(1-b_1)}{(N_{Sc})_1}\left[1 - \frac{B_2}{r_{12}+1}(r_{12}\,a_1 + b_1)\right]}{(N_{Sc})_2\,b_1^{\,2}\,(V_w^+)^2} \tag{53}$$

Solving Equations (42) and (43) simultaneously,

$$\frac{da_1}{dx^+} = \frac{f_3g_2 - f_2g_3}{f_1g_2 - f_2g_1} \tag{54}$$

$$\frac{db_1}{dx^+} = \frac{f_1g_3 - f_3g_1}{f_1g_2 - f_2g_1} \tag{55}$$

The problem now reduces to the simultaneous solution of Equations (25), (54) and (55) for the initial conditions, $\delta^+ = 0$, $a_1 = b_1 = 1$ at $x^+ = 0$. In order to avoid indeterminate values for the derivatives of $\frac{d\delta^+}{dx^+}$, $\frac{da_1}{dx^+}$ and $\frac{db_1}{dx^+}$ at $x^+ = 0$, asymptotic expressions (small x^+) for δ^+, a_1 and b_1 are needed. These will be developed as follows:

The asymptotic expression for δ^+ is given in (9),

$$\delta^+ = 30^{1/2} (x^+)^{1/2} \tag{56}$$

For small x^+, $\overline{U}^+ \approx 1$, $a_1 \approx 1$, $b_1 \approx 1$.

So that A_1^+ may be approximated by (from Equation (34))

$$A_1^+ = \frac{2(a_1 - 1)}{B_1 (1 - B_2)} \tag{57}$$

Substituting Equation (57) into Equation (40) and neglecting the term containing V_w^+, one can obtain, by simple integration, the following asymptotic expression for a_1:

$$a_1 = 1 + \left[\frac{3}{2} \frac{1}{(N_{Sc})_1} \right]^{1/3} B_1 (1 - B_2) \delta^{+1/3} x^{+1/3} \tag{58}$$

A similar derivation yields the asymptotic expression for b_1.

$$b_1 = 1 + \left[\frac{3}{2} (N_{Sc})_2^2 \right]^{1/3} B_1 (1 - B_2) \frac{\delta^{+1/3} x^{+1/3}}{(N_{Sc})_1} \tag{59}$$

The computation proceeds as follows: The system parameters B_1, B_2, N_{Sc_1}, N_{Sc_2}, and r_{12} are first specified. The starting values for arbitrarily small

x^+ are obtained from Equations (56), (58) and (59). Equations (25), (54) and (55) are now solved simultaneously using the Runge Kutta method. At each stage of the computation the value of δ^+, a_1, b_1, Δ_1^+, Δ_2^+, $\overline{U}^+$, V_w^+, as well as the production rate, are obtained. The values of δ^+, a_1 and b_1 are obtained directly from the numerical solution of Equations (25), (54) and (55). $\overline{U}$, Δ_1^+, Δ_2^+, V_w^+ are obtained from Equations (24), (34), (35) and (19) respectively.

The production rate per unit width of membrane is given as:

$$Q = \int_o^x V_w \, dx \tag{60}$$

The dimensionless counterpart of Q, which represents the fraction of water withdrawn, Q^+, is given as:

$$Q^+ = \frac{Q}{bU_o} = \int_o^{x^+} V_w^+ \, dx^+ \tag{61}$$

The integral is evaluated using Simpson's rule.

The numerical solution proceeds until $\delta^+ = 1$. In order to continue the solution the scheme is readily modified by setting $\delta^+ = 1$; $\frac{d\delta^+}{dx^+} = 0$, and solving Equations (54) and (55) simultaneously. The solution is continued until one of the boundary layers, say $\Delta_2^+ = 1$. The rate of growth of boundary layers will, of course, depend on the Schmidt numbers. If the Schmidt number of species 1 is assumed to be greater than that of the second species, Δ_2^+ will reach unity first.

For this region ($\Delta_2^+ = 1$, $0 \leq \Delta_1^+ \leq 1$) it is seen that the equations pertaining to the first component remain unchanged. Different expressions, however, need to be developed for the second component. The integrated form of diffusion equation for the second solute is given as:

$$\frac{d}{dx^+} \int_0^1 u^+ c_2^+ \, dy^+ + V_w^+ (C_2^+)_w = - \frac{1}{N_{Sc_2}} \left(\frac{\partial C_2^+}{\partial y^+}\right)_{y^+=0} \tag{62}$$

C_2^+ can be expressed by the quadratic expression:

$$C_2^+ = b_1 + b_2 y^+ + b_3 y^{+2} \tag{63}$$

Using the symmetry condition $\frac{\partial C_2^+}{\partial y^+} = 0$ at $y^+=1$, one gets:

$$b_3 = - \frac{b_2}{2} \tag{64}$$

The relationship between b_2 and b_1 can be established from the boundary condition of Equation (16). Substituting Equation (63) into Equation (16), one has:

$$b_2 = B_1 \frac{(N_{Sc})_2}{(N_{Sc})_1} \; b_1 \left[\frac{B_2}{r_{12}+1} (r_{12} a_1 + b_1) - 1\right] \tag{65}$$

Combining Equations (23) (with $\delta^+=1$), (63),(64) and (65) and after rearrangement, the following equation results:

$$\ell_1 = \frac{da_1}{dx^+} + \ell_2 \frac{db_1}{dx^+} = \ell_3 \tag{66}$$

where

$$\ell_1 = \frac{4}{15} \frac{(N_{Sc})_2}{(N_{Sc})_1} \; \frac{b_1 \; r_{12}}{r_{12} + 1} \tag{67}$$

$$\ell_2 = \frac{4}{15} B_1 \frac{(N_{Sc})_2}{(N_{Sc})_1} \left[\frac{B_2}{r_{12}+1} (r_{12} a_1 + 2b_1) - 1\right] \tag{68}$$

$$\ell_3 = -\frac{b_2}{N_{Sc_2}} - b_1 V_w^+ \tag{69}$$

The governing equations are now Equations (42) and (66), i.e.

$$\frac{da_1}{dx^+} = \frac{f_3\ell_2 - f_2\ell_3}{f_1\ell_2 - f_2\ell_1} \tag{70}$$

$$\frac{db_1}{dx^+} = \frac{f_1\ell_3 - f_3\ell_1}{f_1\ell_2 - f_2\ell_1} \tag{71}$$

Equations (70) and (71) are now solved simultaneously and the solution can be continued until $\Delta_1^+ = 1$.

RESULTS AND DISCUSSION

As an illustration, the system NaCl - KCl - water was studied in detail (with NaCl designated as solute 1 and Kcl as 2). The Schmidt numbers are 560 and 385 respectively. The following values of B_1, B_2 and r_{12} were considered.

B_1 = 7.4074, 20.0 and 40.0*

B_2 = 0.5, 0.25 and 0

r_{12} = 0.1, 0.5, 1.0 and 10.0

Typical results are presented in Figures 2-5.

In Figure 2, the variations of $(C_1)_w^+$ and $(C_2)_w^+$ vs the dimensionless longitudinal distance, x^+, for the case of $B_1 = 7.4074$, $B_2 = 0.5$ and $r_{12} = 1.0$ are shown. Also included on the same plot is the change of total wall concentration, C_w^+, with x^+. C_w^+ is defined as:

*These values correspond to membrane capacities of 5 gal./day-sq.ft. to 50 gal./day-sq.ft. for brine operating at 100 atm. and a membrane spacing of 0.1 in.

$$C_w^+ = \frac{r_{12}\, a_1 + b_1}{r_{12} + 1} \quad . \tag{72}$$

Figure 3 shows the effect of the parameter r_{12}. The dotted line represents the change in the overall wall concentration C_w^+. It is seen that it is much closer to $(C_1^+)_w$ curve and a check with reference (9) indicates that the results for the case $r_{12} = 10$ are very close to the single component case, $N_{Sc} = 560$.

Figures 4 and 5 present typical results for the variation of the dimensionless wall flux and the fraction of water withdrawn along the axial distance.

Mass transfer characteristics can be defined in the conventional way in terms of the mass transfer coefficient, defined as follows:

$$(K_j)_x = \frac{-D_{jj} \left(\frac{\partial C_j}{\partial y}\right)_{y=0}}{(C_j)_w - (C_j)_b} \quad , \quad j = 1,2 \tag{73}$$

The Sherwood number, $(N_{Sh})_j$, thus becomes:

$$(N_{Sh})_j = \frac{-(\partial C_j^+ / \partial y^+)_{y^+=0}}{(C_j^+)_w - (C_j^+)_b} \quad , \quad j = 1,2 \tag{74}$$

A simple mass balance indicates that

$$(C_j^+)_b = \frac{1}{1 - Q^+} \tag{75}$$

Using the concentration profiles to evaluate $(\partial C_j^+ / \partial y^+)_{y+=0}$, the expressions for the Sherwood number, $(N_{Sh})_j$, are:

$$(N_{Sh})_1 = \frac{(a_1)\,(N_{Sc})_1\,(V_w^+)\,(1 - Q^+)}{a_1\,(1 - Q^+) - 1} \tag{76}$$

$$(N_{Sh})_2 = \frac{(b_1)\,(N_{Sc})_2\,(V_w^+)\,(1 - Q^+)}{b_1\,(1 - Q^+) - 1} \tag{77}$$

A typical plot of $(N_{Sh})_j$ vs x^+ is shown in Figure 6. Additional results are presented in Tables 1-6. It is worthwhile to note that although the concentration polarization is substantially affected by the presence of a second solute, the Sherwood number is found to be less affected. In terms of practical application, the difference in N_{Sh} for various values of r_{12} is sufficiently small that one can very well use the information on N_{Sh} obtained from the binary system for the study of multicomponent cases.

The results of the present analysis can also be used for the prediction of the conditions under which a given species of solution can be precipitated out. As an illustration, consider the system of KCl - $CaSO_4$ - H_2O. The Schmidt numbers are 385 and 610 respectively, and the initial concentration of $CaSO_4$ is assumed to be 0.01 gm.mols/liter, $r_{12} = 1$ and $B_2 = 0.5$. Here component 1 refers to $CaSO_4$. The saturation concentration of $CaSO_4$ is 0.0154 gm.mols/liter and hence when the dimensionless wall concentration (C_1^+) is 1.54, the salt would tend to precipitate. Figure 7 shows the plot of wall concentrations vs. x^+. It is seen that when $x^+ = 3.9$, $(C_1^+)_w = 1.54$. If the membrane spacing, $2b$, is 1/4 inch and the inlet Reynolds number based on equivalent diameter, $4N_{Re_i}$, is 1200, the maximum length of the duct without precipitation would correspond to (300)(1/96)(3.9) = 12.2 ft. At this length, $CaSO_4$ would tend to separate out. A similar calculation for the system NaCl - $CaSO_4$ - H_2O yields a value of $x^+ = 5.85$ which, for the dimensions of the duct discussed above and an inlet Reynolds number of 1200, corresponds to (300)(1/96)(5.85) = 18.3 ft.

The plot of wall concentrations vs. x^+ is shown in Figure 8.

It must be pointed out that although the ternary case has been considered (two components in solution), the present analysis can be extended to systems of n components in solution. In this case, V_w^+ is given by:

$$V_w^+ = \frac{B_1}{(N_{Sc})_1}\left[1 - B_2 \frac{\sum_{j=1}^{N} (C_j^+)_w / r_{1j}}{\sum_{j=1}^{N} 1 / r_{1j}}\right] \tag{78}$$

where $r_{11} = 1$.

The derivations follow as in the case of the ternary system.

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LITERATURE CITED

1. Brian, P.L.T., Ind. Eng. Chem. Fundamentals, 4, 439 (1965).

2. Dresner, L., Oak Ridge National Laboratory Report No. ORNL 3621 (May 1964).

3. Fisher, R.E., T.K. Sherwood and P.L.T. Brian, M.I.T. Report No. 295-5 DSR 9336 (1965).

4. Gill, W.N., C. Tien and D.W. Zeh, Ind.Eng.Chem.Fundamentals 4, 433 (1965).

5. Gill, W.N., C. Tien and D.W. Zeh, Int.J.Heat and Mass Transfer 9, 907 (1966).

6. Gill, W.N., C. Tien and D.W. Zeh, A.I.Ch.E.Journal 12, 1141 (1966).

7. Nakano, Y., C. Tien and W.N. Gill, A.I.Ch.E. Journal 13, 1092 (1967).

8. Sherwood, T.K., P.L.T. Brian, R.E. Fisher and R.L. Dresner, Ind.Eng. Chem. Fundamentals 4, 113 (1965).

9. Srinivasan, S., C. Tien, W.N. Gill, Chem. Eng. Sci. 22, 417 (1967).

10. Srinivasan, S., and C. Tien, Desalination 3, 5 (1967).

11. Srinivasan, S. and C. Tien, "A Finite Difference Solution for Reverse Osmosis in Turbulent Flow", (To be published).

12. Tien, C. and W.N. Gill, A.I.Ch.E. Journal 12, 722(1966).

NOMENCLATURE

A	Membrane constant
a_1, a_2, a_3	Coefficients in the concentration profile for solute 1 (Equation 28)
b	half distance between membrane sheets
b_1, b_2, b_3	Coefficients in the concentration profile for solute 2 (Equation 29)
B_1, B_2	constants defined by Eq. (17) and Eq. (10), respectively
C_1	Concentration of solute 1
C_2	Concentration of solute 2
$(C_1)_o$	Concentration of solute 1 at inlet
$(C_2)_o$	Concentration of solute 2 at inlet
C_1^+	$C_1/(C_1)_o$
C_2^+	$C_2/(C_2)_o$
$(C_j)_b$	Bulk concentration of solute j
$(C_j^+)_b$	$(C_j)_b/(C_j)_o$
$(C_j)_w$	Wall concentration of solute 2
$(C_j^+)_w$	$C_j/(C_j)_o$
$D_{11}, D_{12}, D_{21}, D_{22}$	Diffusivities
f_1, f_2, f_3	Defined by Equations (44-46)
g_1, g_2, g_3	Defined by Equations (49-51)
$(K_j)_x$	Mass transfer coefficient for solute j.
ℓ_1, ℓ_2, ℓ_3	Defined by Equations (67)-(69)
$(N_{Sc})_1, (N_{Sc})_2$	Schmidt numbers
$(N_{Sh})_1, (N_{Sh})_2$	Sherwood numbers

N_{Re_i}	Reynolds number, bU_o/ν , at inlet
P_{os}	Osmotic pressure
$(P_{os})_o$	Osmotic pressure at inlet
P_1, P_2	Defined by Equations (47) (48)
Q	Volumetric production per unit width
Q^+	Fraction of water withdrawn
q_1, q_2	Defined by Equations (52),(53)
r_{1j}	$(C_1)_o/(C_j)_o$
u	Component of velocity in the x-direction
$\overline{U}$	Potential velocity
$\overline{U}^+$	U/U_o
U_o	Average velocity at inlet
u^+	u/U_o
v	Component of velocity in the y-direction
v^+	bV/ν
V_w	Transverse wall velocity
V_w^+	bV_w/ν
x	Axial distance along duct
x^+	$x/b\ N_{Re_i}$
y	Distance normal to x measured from membrane surface
y^+	y/b

Greek Letters

δ	Momentum boundary layer thickness
δ^+	δ/b
Δ_j	Concentration boundary layer thickness for species j
Δ_j^+	Δ/b
ν	Kinematic viscosity

TABLE 1

$B_1 = 7.4074$

	$B_2 = 0.5$ $r_{12} = 0.1$		$B_2 = 0.5$ $r_{12} = 1.0$		$B_2 = 0.5$ $r_{12} = 10$		
x^+	N_{Sh_1}	N_{Sh_2}	N_{Sh_1}	N_{Sh_2}	N_{Sh_1}	N_{Sh_2}	$N_{Sc}=560$ Single Component
0.01	47.1995	43.6791	47.1450	43.6181	47.0913	43.5582	45.9246
0.10	18.6537	17.0836	18.5856	17.0105	18.5210	16.9410	17.7091
0.50	11.2193	10.1386	11.1446	10.0627	11.0773	9.9948	10.9456
1.00	9.0562	8.1637	8.9763	8.0836	8.0967	8.0144	8.8465
5.00	5.5495	4.9962	5.4671	4.9165	5.4016	4.8542	5.3897
10.00	4.5190	4.0868	4.4428	4.0143	4.3847	3.9601	4.3814
20.00	3.70716	3.39577	3.6427	3.3351	3.5955	3.2918	3.60068
30.00	3.3230	3.0897	3.2683	3.0381	3.2291	3.0024	3.24054
40.00	3.0903	2.9211	3.0349	2.8709	3.0026	2.8414	3.02799
50.00	2.9338	2.8234	2.8886	2.7823	2.8674	2.7608	2.8894

TABLE 2

$B_1 = 7.4074$

	$B_2 = 0.25$ $r_{12} = 0.1$		$B_2 = 0.25$ $r_{12} = 1.0$		$B_2 = 0.25$ $r_{12} = 10$		
x^+	N_{Sh_1}	N_{Sh_2}	N_{Sh_1}	N_{Sh_2}	N_{Sh_1}	N_{Sh_2}	$N_{Sc}=560$ Single Component
0.01	48.0193	44.4591	47.9851	44.4211	47.9513	44.3852	46.2834
0.10	19.5293	17.8931	19.4710	17.8305	19.4151	17.7706	17.8605
0.50	12.1239	10.9349	12.0364	10.8449	11.9568	10.7640	11.7444
1.00	9.9705	8.9636	9.8604	8.8512	9.7652	8.7551	9.6678
5.00	6.4185	5.7438	6.2475	5.5695	6.1221	5.4469	6.1002
10.00	5.3147	4.7652	5.1264	4.5734	5.0009	4.4531	4.9928
20.00	4.3818	3.9678	4.1951	3.7758	4.0821	3.6690	4.0896
30.00	3.9013	3.5829	3.7278	3.4002	3.6284	3.3057	3.6480
40.00	3.5878	3.3528	3.4298	3.1796	3.3429	3.0954	3.3732
50.00	3.3516	3.2013	3.2188	3.0407	3.1431	2.9649	3.1834
60.00	3.1882	3.1175	3.0606	2.9542	2.9952	2.885	3.0453
70.00	3.0625	3.1152	2.9371	2.9062			

TABLE 3

$B_1 = 20$

	$B_2 = 0.5$ $r_{12} = 0.1$		$B_2 = 0.5$ $r_{12} = 1.0$		$B_2 = 0.5$ $r_{12} = 10$		
x^+	N_{Sh_1}	N_{Sh_2}	N_{Sh_1}	N_{Sh_2}	N_{Sh_1}	N_{Sh_2}	$N_{Sc}=560$ Single Component
0.01	48.4810	44.6737	48.2778	44.4518	48.0860	44.2429	45.6081
0.10	19.5215	17.6324	19.2648	17.3729	19.0500	17.1579	17.2430
0.50	11.7765	10.3931	11.5514	10.1898	11.3777	10.0355	11.0697
1.00	9.4709	8.3077	9.2643	8.1277	9.1098	7.9954	8.9694
5.00	5.6956	4.9632	5.5543	4.8518	5.4527	4.7726	5.4289
10.00	4.5906	4.0175	4.4801	3.9345	4.4013	3.8759	4.3944
20.00	3.7284	3.3086	3.6482	3.2518	3.5914	3.2118	3.5975
30.00	3.3247	2.9986	3.2620	2.9564	3.2179	2.9269	3.2322
40.00	3.0822	2.8295	3.0321	2.7977	2.9884	2.7703	3.0178
50.00	2.9139	2.7297	2.8805	2.7096	---	---	2.8793

TABLE 4

$B_1 = 20$

	$B_2 = 0.25$ $r_{12} = 0.5$		$B_2 = 0.25$ $r_{12} = 1.0$		$B_2 = 0.25$ $r_{12} = 10$		
x^+	N_{Sh_1}	N_{Sh_2}	N_{Sh_1}	N_{Sh_2}	N_{Sh_1}	N_{Sh_2}	$N_{Sc}=560$ Single Component
0.01	50.7918	46.8636	50.7216	46.7865	50.5547	46.6033	46.6928
0.10	21.8658	19.7189	21.7102	19.5561	21.3776	19.2133	17.9493
0.50	13.8038	11.9939	13.6173	11.8232	13.2561	11.5008	12.5784
1.00	11.2772	9.6760	11.0917	9.5149	10.7450	9.2215	10.4232
5.00	6.8847	5.7719	6.7492	5.6722	6.5019	5.4908	6.4442
10.00	5.5149	4.6161	5.4087	4.5432	5.2139	4.4084	5.1951
20.00	4.3998	3.7171	4.3219	3.6670	4.7189	3.5742	4.1897
30.00	3.8516	3.3007	3.7900	3.2628	3.6769	3.1928	3.70503
40.00	3.5065	3.0566	3.4564	3.02704	3.3646	2.9727	3.4063
50.00	3.2644	2.9018	3.2233	2.8784	3.1481	2.8362	3.2018
60.00	3.0764	2.7996	3.0432	2.7814	2.9894	2.7525	3.0544

TABLE 5

$B_1 = 40$

	$B_2 = 0.25$ $r_{12} = 0.5$		$B_2 = 0.25$ $r_{12} = 1.0$		$B_2 = 0.25$ $r_{12} = 10$		
x^+	N_{Sh_1}	N_{Sh_2}	N_{Sh_1}	N_{Sh_2}	N_{Sh_1}	N_{Sh_2}	$N_{Sc}=560$ Single Component
0.01	54.7782	50.2117	54.5135	49.9212	53.9239	49.2798	46.7064
0.05	30.5041	27.1804	30.0864	26.7547	29.2754	25.9514	22.9987
0.10	23.9653	20.9141	23.5418	20.5179	22.7580	19.8049	17.0749
0.50	14.6881	12.1937	14.3915	11.9775	13.8454	11.5803	12.5929
1.00	11.8199	9.7027	11.5822	9.5404	11.1172	9.2167	10.5305
5.00	7.0219	5.6987	6.8775	5.6086	6.6076	5.4380	6.5163
10.00	5.5804	4.5463	5.4713	4.4807	5.2671	4.3565	5.2369
20.00	4.4223	3.6520	4.3447	3.6077	4.1995	3.5243	4.2082
30.00	3.8577	3.2373	3.7974	3.2048	3.6846	3.1438	3.7133
40.00	3.5040	2.9937	3.4557	2.9694	3.3655	2.92418	3.4088
50.00	3.2568	2.8387	3.2178	2.8207	3.1449	2.7878	3.2009
60.00	3.0735	2.7399	3.04216	2.7270	2.9837	2.7041	3.0513

TABLE 6

$B_1 = 40$

	$B_2 = 0.5$ $r_{12} = 0.1$		$B_2 = 0.5$ $r_{12} = 1.0$		$B_2 = 0.5$ $r_{12} = 10$		
x^+	N_{Sh_1}	N_{Sh_2}	N_{Sh_1}	N_{Sh_2}	N_{Sh_1}	N_{Sh_2}	$N_{Sc}=560$ Single Component
0.01	49.9757	45.7034	49.4516	45.1466	48.9948	44.6659	44.8385
0.05	26.1349	23.4053	25.6009	22.8842	25.1879	22.4884	22.1358
0.10	20.0714	17.7622	19.5909	17.3205	19.2334	16.9974	16.0916
0.50	11.9951	10.3377	11.6811	10.0929	11.4522	9.9156	10.9817
1.00	9.5989	8.2275	9.3378	8.0318	9.1494	8.8912	8.9375
5.00	5.7182	4.8908	5.5644	4.7856	5.4542	4.7098	5.4208
10.00	4.5958	3.9574	4.4803	3.8816	4.3971	3.8269	4.3864
20.00	3.7244	3.2596	3.6427	3.2096	3.5844	3.1737	3.5894
30.00	3.3178	2.9548	3.2550	2.9192	3.2105	2.8938	3.2244
40.00	3.0743	2.7892	3.0248	2.7638	2.9898	2.7459	3.0106
50.00	2.9124	2.6955	---	---	---	---	2.8728

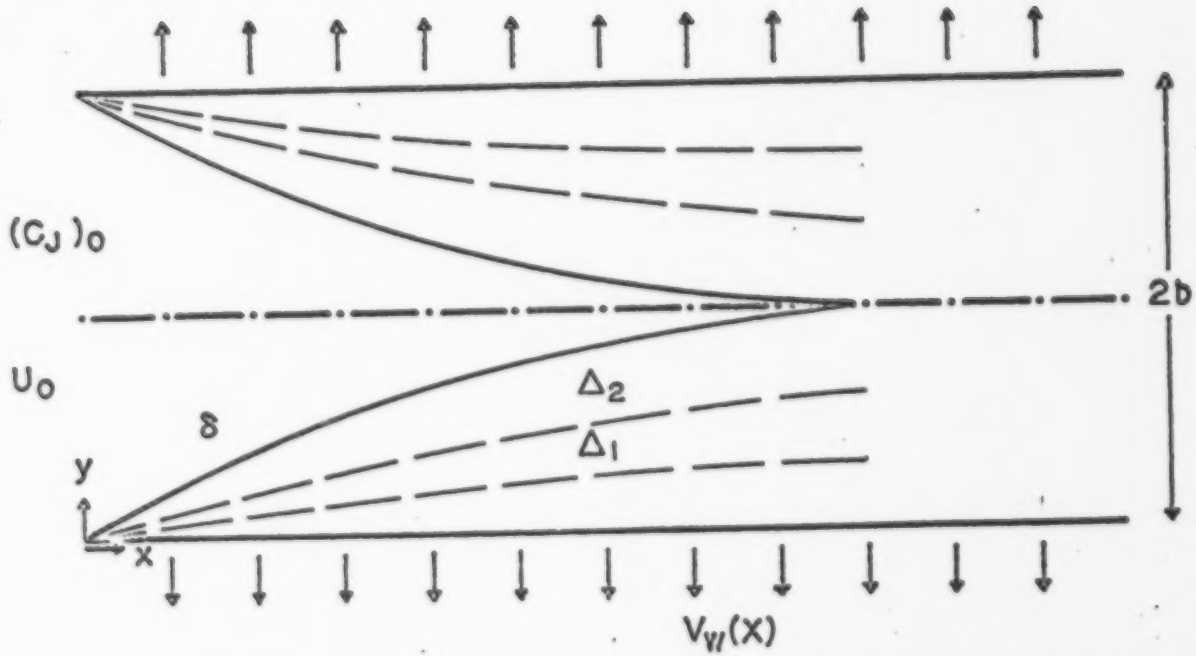

FIG. 1 SCHEMATIC DIAGRAM OF REVERSE OSMOSIS DUCT

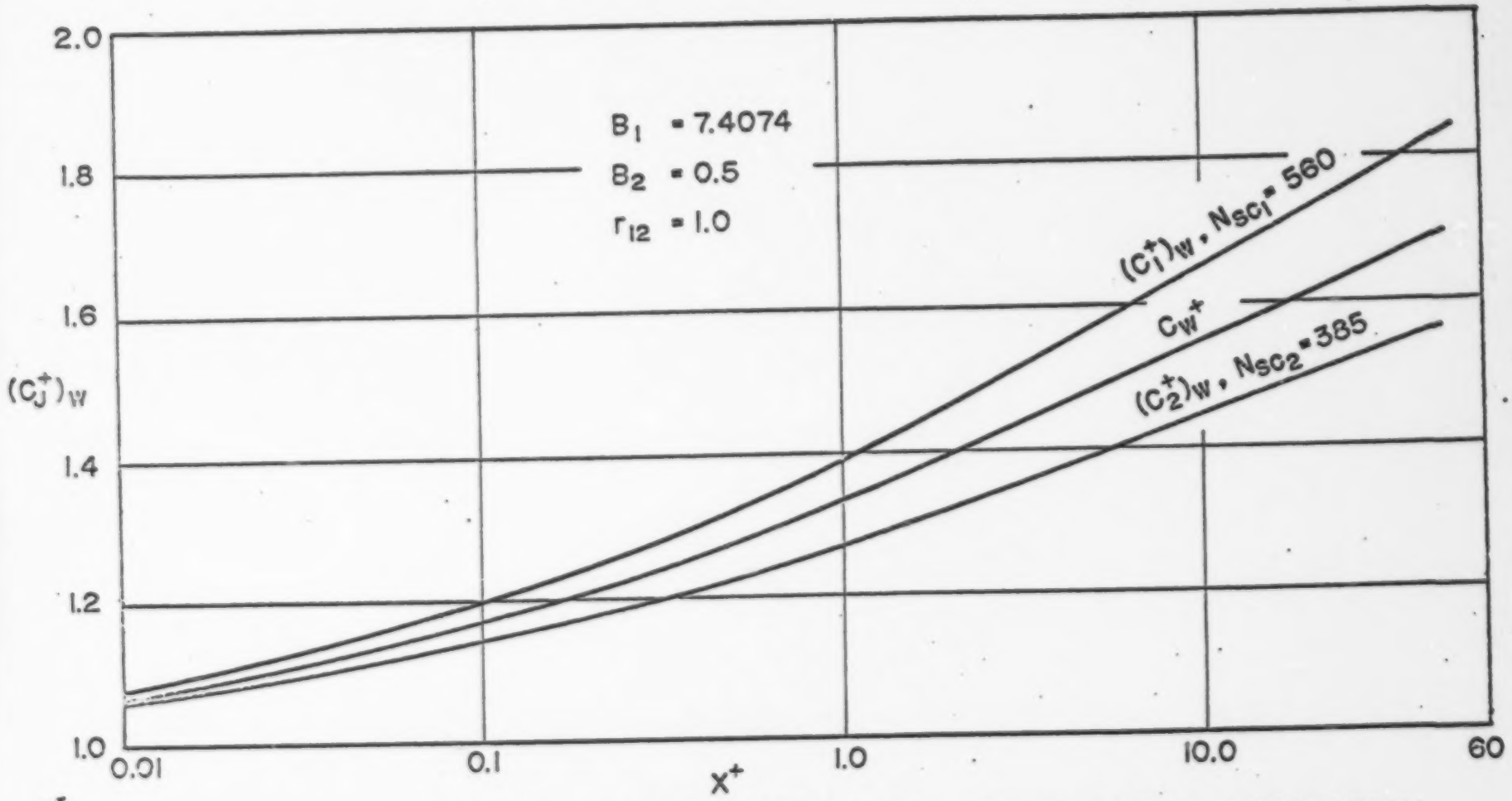

FIG. 2 DIMENSIONLESS WALL CONCENTRATIONS VS. DIMENSIONLESS LONGITUDINAL DISTANCE

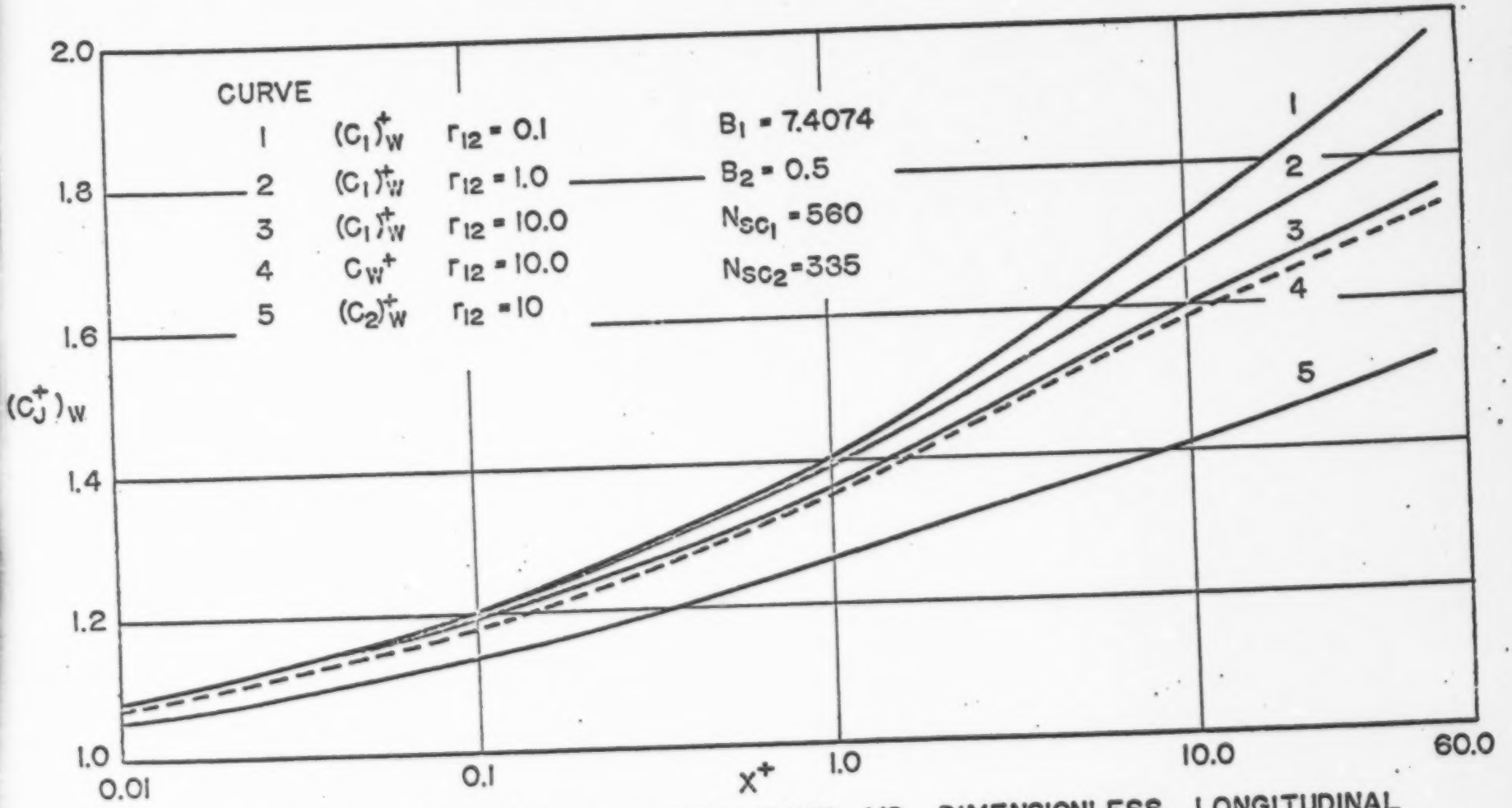

FIG. 3 DIMENSIONLESS WALL CONCENTRATIONS VS. DIMENSIONLESS LONGITUDINAL DISTANCE

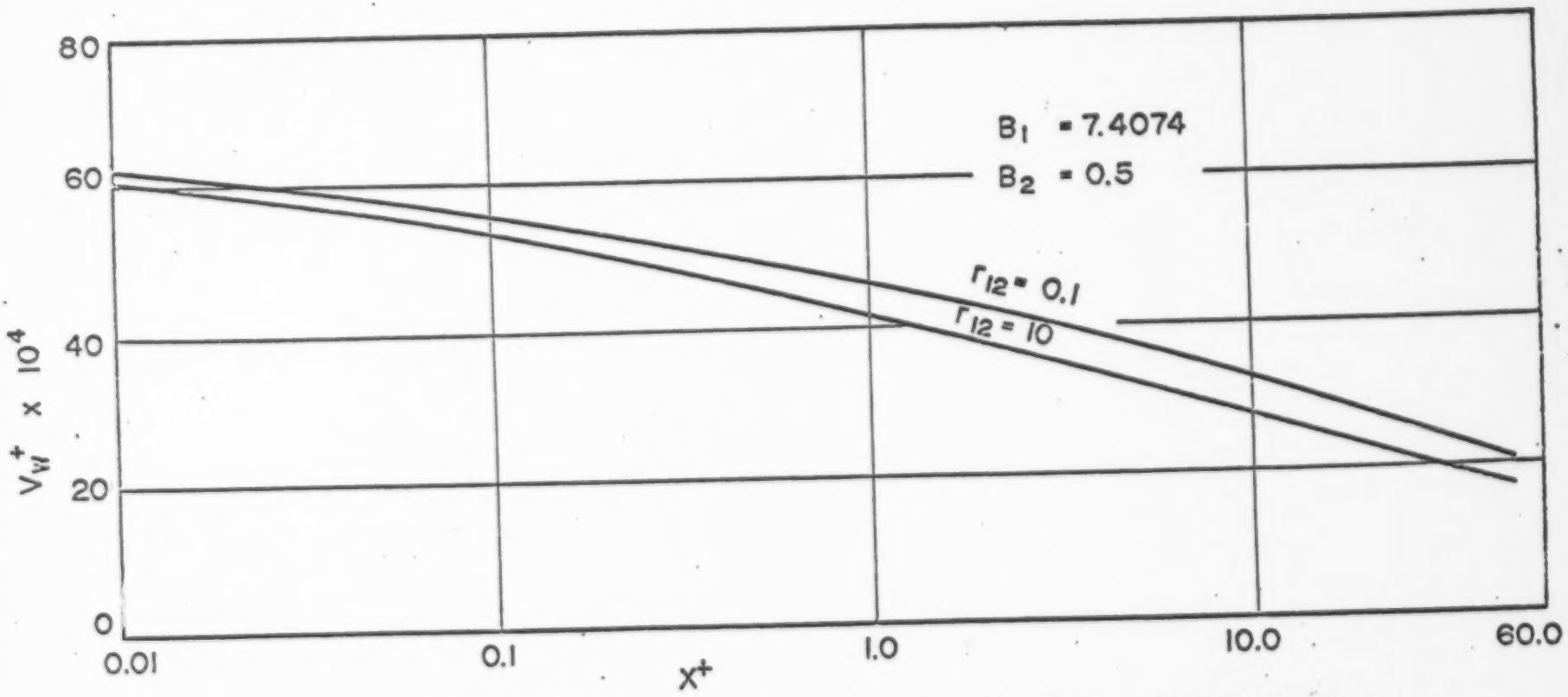

FIG. 4 DIMENSIONLESS WALL VELOCITY VS. DIMENSIONLESS LONGITUDINAL DISTANCE

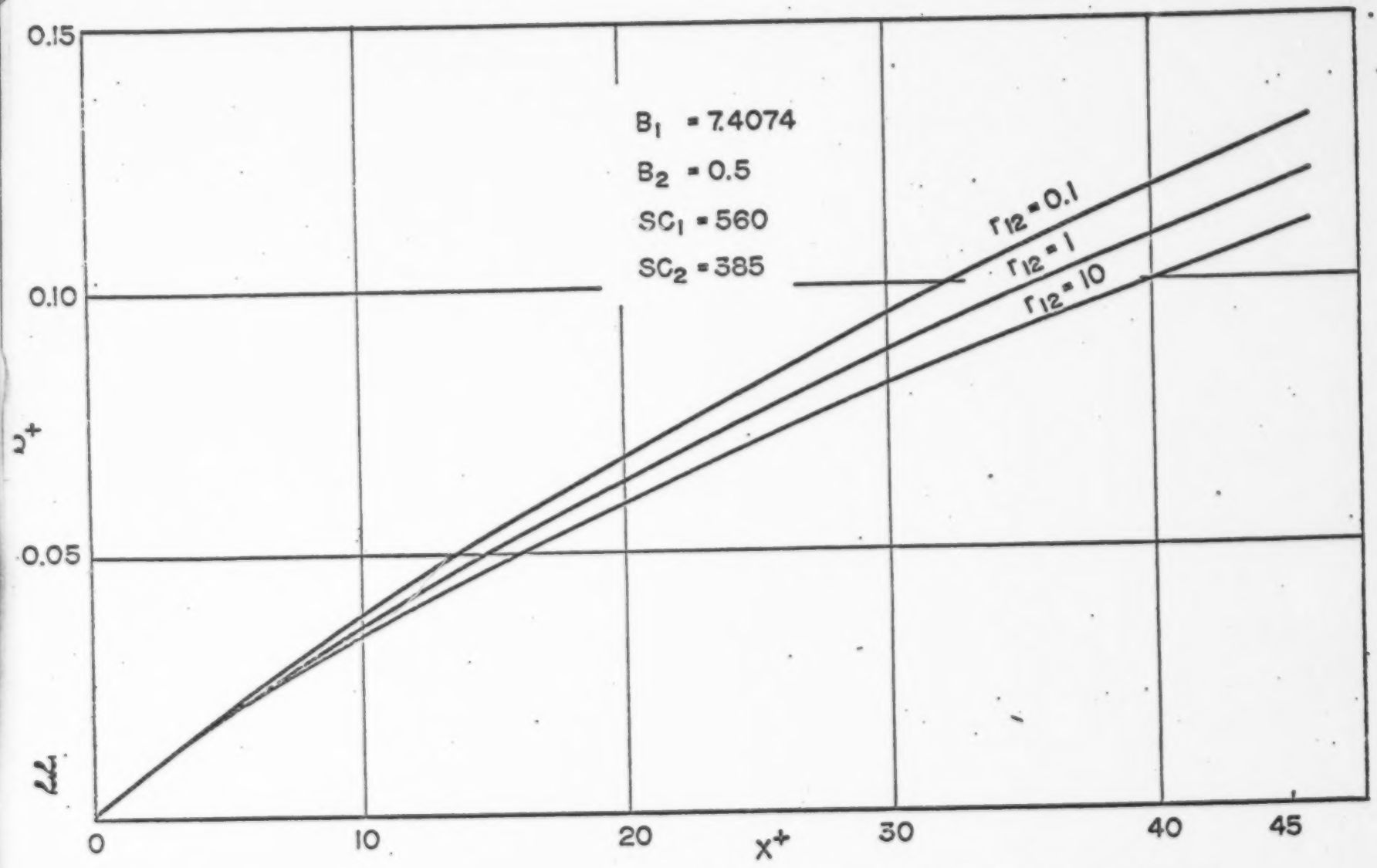

FIG. 5 FRACTION OF WATER WITHDRAWN VS. DIMENSIONLESS LONGITUDINAL DISTANCE

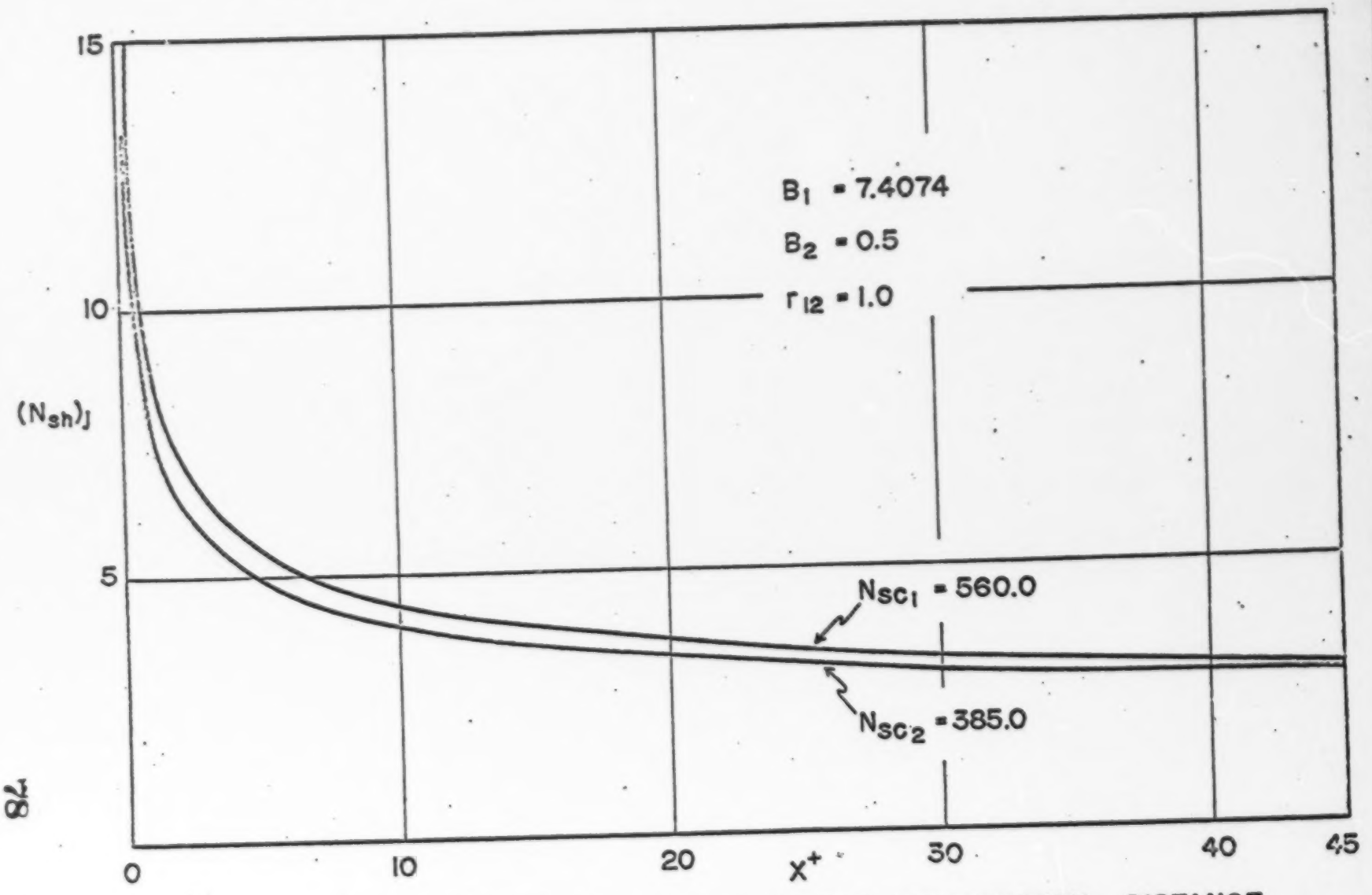

FIG. 6 SHERWOOD NUMBERS VS. DIMENSIONLESS LONGITUDINAL DISTANCE

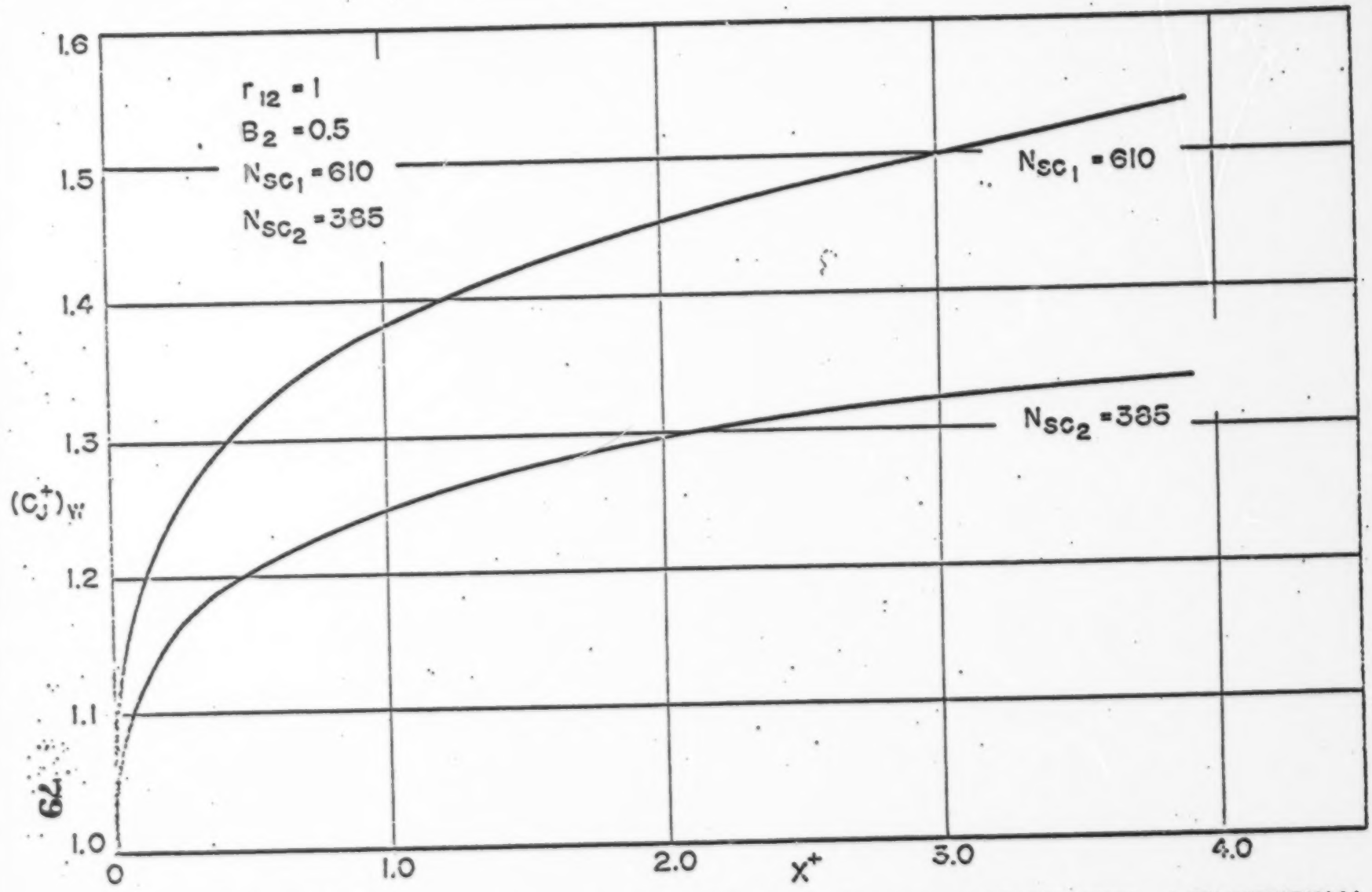

FIG. 7 DIMENSIONLESS WALL CONCENTRATIONS VS. DIMENSIONLESS LONGITUDINAL DISTANCE

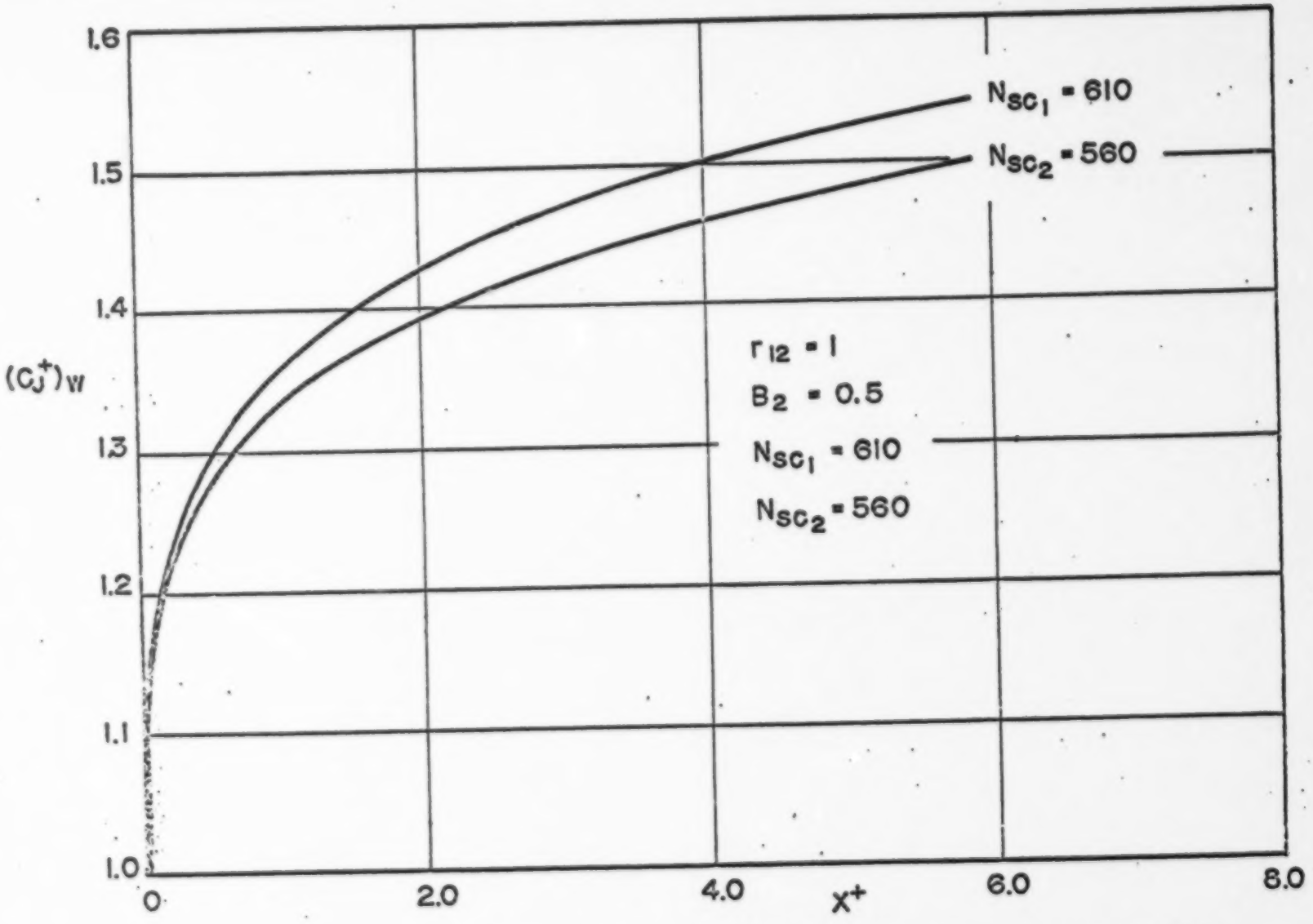

FIG. 8 DIMENSIONLESS WALL CONCENTRATIONS VS. DIMENSIONLESS LONGITUDINAL DISTANCE

A SIMPLIFIED METHOD FOR THE PREDICTION OF CONCENTRATION POLARIZATION IN REVERSE OSMOSIS OPERATION FOR MULTICOMPONENT SYSTEMS

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ABSTRACT

A simplified procedure is presented for the prediction of concentration polarization in reverse osmosis operation where a multicomponent stream is treated, by using the information obtained from one-solute system. The method which is based on the observation that the local Sherwood number for a given species of solution is approximately proportional to the cubic root of its Schmidt number and relatively independent of other parameters, involves the simultaneous solution of n coupled integral equations. The method is tested for two- and three-solute systems and the results are compared with those obtained from the more rigorous method. Good agreements are observed for both cases.

INTRODUCTION

Accurate prediction of concentration build-up along membrane surface is of paramount importance for the proper design of reverse osmosis system and has been a subject of considerable interest (1-4). Most of the investigations, however have been confined to one-solute systems with the exception of the recent work of Srinivasan and Tien (5), which considered the ternary systems, i.e. (two solutes). In all these studies, the concentration polarization is predicted through the simultaneous solution of equations of motion and diffusion with appropriate boundary conditions.

In actual application of reverse osmosis, the feed stream can hardly be described as one-solute system. In the case of waste water renovation, several species of salts of comparable concentration are present. Furthermore, in order to determine the need of pretreatment for the prevention of precipitates of certain solutes, one should include even those solutes which are in minute quantities in the consideration of the concentration polarization of the system.

In principle, one can obtain the necessary information on concentration build-up through the simultaneous solution of the pertinent equations. However, with a large number of solutes under consideration, complexities increase accordingly and there is a practical limit as to the number of solutes which can be considered. There is need to devise a simple alternative, which is the object of the present work.

In this investigation, we shall present a simple method for the prediction of concentration polarization in reverse osmosis for multicomponent systems. The method is based on the observation that even though that the concentration polarization for individual salt changes drastically with the presence of other salts, the mass transfer characterization in terms of local Sherwood number remains essentially to be a function of the Schmidt number of the respective solute

and is only weakly dependent upon other parameters. Consequently, it is possible, as a first order of approximation to devise a procedure for the calculation of concentration polarization of multicomponent system based on the information of single solute system.

In the following sections, a brief description of this procedure is presented, followed with working examples to demonstrate the accuracy of the proposed method.

ANALYSIS

A. Two-Solute System

We shall first demonstrate the procedure for the case where the feed stream consists of two solutes. The permeation velocity, V_w, of pure water across the membrane can be described by the following phenomenological law:

$$|V_w| = A(\Delta p - \pi_{os}) \tag{1}$$

where A is the membrane constant, Δp is the pressure difference across the membrane and π_{os} is the osmotic pressure corresponding to the concentration prevailing at the membrane surface. Equation (1) is written on the basis that the membrane is perfect. One can introduce a rejection ratio to the above expression for a more realistic situation.

If ideal solution behavior is assumed for the two-solute system, the osmotic pressure can be considered as a linear function of total concentration* [Equation (1)] can be written as

$$|V_w| = A(\Delta p)\left[1 - B_2 \frac{(C_1)_w + (C_2)_w}{(C_1)_o + (C_2)_o}\right] \tag{2}$$

$$B_2 = \frac{(\pi_{os})_o}{\Delta p} \tag{3}$$

*Both concentrations are given in terms of milliequivalent.

where $(\pi_{os})_o$ is the osmotic pressure at concentration of $(C_1)_o + (C_2)_o$.

In term of dimensionless form, Equation (3) can be rewritten as

$$|V_v^*| = \frac{|V_v|b}{\nu} = \frac{B_1}{R_{3c_1}}\left[1 - B_2 \frac{r_{12}(C_1^*)_w + (C_2^*)_w}{r_{12} + 1}\right] \tag{4}$$

where

$$B_1 = \frac{(\lambda)(\Delta\pi)b}{D_{11}} \tag{5}$$

$$r_{12} = \frac{(C_1)_o}{(C_2)_o} \tag{6}$$

and b is the characteristic length of the membrane conduit.

The fractional of water recovered, Q^*, is usually defined as

$$Q^* = \frac{Q}{bU_o} = \int_o^{x^*} V_v^* \, dx^* \tag{7}$$

where x^* is the dimensionless distance measured along the longitudinal direction of the membrane duct.

Based on the assumption that the cross diffusion terms are negligible, the mass transfer coefficient for the two solutes can be written as

$$(k_j)_{x^*} = \frac{-D_{jj}\left(\frac{\partial C_j}{\partial y}\right)_{y=0}}{(C_j)_w - (C_j)_b}, \quad j = 1,2 \tag{8}$$

where y is the distance away from the membrane surface.

The condition of product side vaporation can be written as

$$-D_{jj}\left(\frac{\partial C_j}{\partial y}\right)_o = (V_w)(C_j)_w \quad j = 1,2 \tag{9}$$

The left side function, $(C_j)_o^*$ of a given species can be combined from Eq. (8) to (9) to obtain

$$(C_j)_o^* = \frac{C_j}{(C_j)_w} \tag{10}$$

The local Sherwood number is conventionally defined as

$$(N_{Sh})_j = \frac{(k_j)_x \, b}{D_{jj}} \tag{11}$$

Combining Equations (8), (10) and (11), one has

$$(N_{Sh})_1 = \frac{(k_1)_x \, b}{D_{11}} = \frac{(N_{Sc})_1 \, (a_1) \, (V_w^+) \, (1-Q^+)}{a_1(1-Q^+) - 1} \tag{12a}$$

$$(N_{Sh})_2 = \frac{(k_2)_x \, b}{D_{22}} = \frac{(N_{Sc})_2 \, (a_2) \, (V_w^+) \, (1-Q^+)}{a_2(1-Q^+) - 1} \tag{12b}$$

where a_1 and a_2 denote $(C_1^+)_w$ and $(C_2^+)_w$, respectively.

Equations (12a) and (12b) may be written as

$$r_{12} \int_o^{x^+} a_1 dx^+ + \int_o^{x^+} a_2 dx^+ = \frac{1}{\beta} \left[\alpha x^+ + \frac{(N_{Sh})_1}{G_1} - 1 \right] \tag{13a}$$

$$r_{12} \int_o^{x^+} a_1 dx^+ + \int_o^{x^+} a_2 dx^+ = \frac{1}{\beta} \left[\alpha x^+ + \frac{(N_{Sh})_2}{G_2} - 1 \right] \tag{13b}$$

where

$$\alpha = \frac{B_1}{(N_{Sc})_1} \tag{14}$$

$$\beta = \frac{B_1 B_2}{(N_{Sc})_1 \, (r_{12} + 1)} \tag{15}$$

$$G_1 = a_1 \left[(N_{Sh})_1 - (N_{Sc})_1 \, (V_w^+) \right] \tag{16}$$

$$G_2 = a_2 \left[(N_{Sh})_2 - (N_{Sc})_2 \, (V_w^+) \right] \tag{17}$$

Differentiating Equation (13a) with respect to x^+, one has

$$\frac{d}{dx^+} \left[\frac{(N_{Sh})_1}{G_1 \beta} \right] = r_{12} \, a_1 + a_2 - \alpha/\beta \tag{18}$$

After straightforward differentiation and rearrangement, Equation (18) may be written as follows:

$$f_1 \frac{da_1}{dx^*} + f_2 \frac{db_1}{dx^*} = f_3 \tag{19}$$

where

$$f_1 = \frac{(N_{Sh})_1}{G_1^2 \beta} \left[(N_{Sh})_1 + (N_{Sc})_1 (a_1/\beta)(x_{12}) - (N_{Sc})_1 (\nu_w^*) \right] \tag{20}$$

$$f_2 = \frac{(N_{Sh})_1 (N_{Sc})_1 (a_1)}{G_1^2} \tag{21}$$

$$f_3 = \frac{\left[G_1 - (N_{Sh})_1 (a_1) \right]}{G_1^2 \beta} \frac{d(N_{Sh})_1}{dx^*} - \left[x_{12} c_1 + c_2 - a/\beta \right] \tag{22}$$

A similar treatment of Equation (18b) yields,

$$g_1 \frac{da_1}{dx^*} + g_2 \frac{da_2}{dx^*} = g_3 \tag{23}$$

where

$$g_1 = \frac{(N_{Sh})_2 (N_{Sc})_2 (a_2)(x_{21})}{G_2^2 \beta} \tag{24}$$

$$g_2 = \frac{(N_{Sh})_2}{G_2^2 \beta} \left[(N_{Sh})_2 + (N_{Sc})_2 (a_2/\beta) + (N_{Sc})_2 (\nu_w^*) \right] \tag{25}$$

$$g_3 = \left[\frac{G_2 - (N_{Sh})_2 c_2}{G_2^2 \beta} \right] \frac{d(N_{Sh})_2}{dx^*} - \left[x_{21} c_1 + c_2 - c/\beta \right] \tag{26}$$

The solution of Equations (19) and (23) are:

$$\frac{da_1}{dx^*} = \frac{f_3 g_2 - g_3 f_2}{f_1 g_2 - g_1 f_2} \tag{27}$$

$$\frac{da_2}{dx^*} = \frac{f_1 g_3 - g_1 f_3}{f_1 g_2 - g_1 f_2} \tag{28}$$

The estimation of the concentration polarization of species 1 and 2 can be made by the simultaneous solution of Equations (27) and (28) provided that the dependence of the local Sherwood number on the longitudinal distance of the membrane duct is known. On the other hand, it has been demonstrated previously (5) that the local Sherwood number is approximately proportional to the 1/3 power of the Schmidt number and, furthermore, for a given species of solute the variation of (N_{Sh}) along x^* for a multicomponent system remains essentially the same as that of one-solute system. Since various aspects of one solute system have been studied rather extensively in the past, $(N_{Sh})_1$ and $(N_{Sh})_2$ can be established from existing literature and used in conjunction with Equations (27) and (28) to obtain the concentration build-up at membrane surface as a function of longitudinal distance.

B. n-Solute System

A general expression for a feed stream containing n species of solutes similar to that given above for two solutes system is now presented. Equation (1) is again used to describe the polarization of pure water across membrane. The assumption that osmotic pressure is a linear function of the concentrations of all species lead to the following expression:

$$\left[v_w\right]_j = A(\Delta p) \left[\lambda - \sum_{i=2}^{n} \sigma_i \frac{\left(c_i\right)_j - \left(c_i\right)_p}{\left(c_i\right)_b - \left(c_i\right)_p} \right] \tag{29}$$

σ_i is defined as before [Equation (1)] and $(c_i)_p$ for the osmotic pressure at the concentration of $(c_i)_j$.

The [illegible] is obtained as

$$[illegible] \tag{30}$$

where [illegible]

$$\beta_n = \frac{B_1 B_2}{(N_{Sc})_1 \prod_{j=1}^{n} \gamma_j} \tag{31}$$

$$\gamma_j = \prod_{\substack{i=1 \\ i \neq j}}^{n} r_{1i} \tag{32}$$

$$r_{1i} = \frac{(C_1)_o}{(C_i)_o} \tag{33}$$

$$B_1 = \frac{A(\Delta\sigma)b}{D_{11}} \tag{34}$$

The fraction of water withdrawn, Q^+, is given as

$$Q^+ = \frac{Q}{bU_o} = \int_o^{x^+} V_w^+ \, dx^+$$

Use the same treatment as before, the counterpart of Equation (18) for component j in a n-solute system is found to be:

$$\frac{d}{dx^+}\left[\frac{(N_{Sh})_j}{G_j \beta_n}\right] = \prod_{j=1}^{n} \gamma_j (a_j) = \frac{a}{\beta_n} \tag{35}$$

$$j = 1, \text{---} \; n$$

and

$$G_j = (N_{Sh})_j (a_j) - (a_j) (N_{Sh})_j V_w^+ \tag{36}$$

After some minor rearrangements, the system of differential equations involving the wall concentrations of all species of solutes can be written as,

$$\begin{bmatrix} f_{11} & f_{12} \cdots & f_{1n} \\ f_{21} \cdots\cdots & & f_{2n} \\ \vdots & & \\ f_{n1} \cdots\cdots & & f_{nn} \end{bmatrix} \begin{bmatrix} da_{11}/dx^+ \\ da_{12}/dx^+ \\ \\ da_{1n}/dx^+ \end{bmatrix} = \begin{bmatrix} f_{1n+1} \\ f_{2n+1} \\ \\ f_{nn+1} \end{bmatrix} \tag{37}$$

where, for $j = 1, \ldots n$:

$$f_{jj} = \frac{(\mu_{jn})_j^2}{c_j^2 \beta_n} \left[(\mu_{nn})_j + (\mu_{ge})_j (e_j) (\gamma_j) - (\mu_{ge})_j (\gamma_n^*) \right] \tag{38a}$$

$$f_{jk} = \frac{(\mu_{jn})_j (\mu_{ge})_k (e_j) (\gamma_k)}{c_j^2} \qquad \begin{matrix} k = 1, \ldots n \\ k \neq j \end{matrix} \tag{38b}$$

$$f_{j,n+1} = \left[c_j - \frac{(\mu_{jn})_j c_{11}}{c_j^2} \right] \frac{d(\mu_{jn})_j}{dx^*} - \sum_{j=1}^{n} \gamma_j (e_{1j}) + \frac{c_1}{\beta_n} \tag{38c}$$

From Equation (37) the functional form of dc_{11}/dx^* through dc_{1n}/dx^* may be readily obtained using Cramer's rule.

$$\frac{dc_{1n}}{dx^*} = \frac{\begin{bmatrix} f_{11} & f_{12} \cdots & f_{1,n+1} \cdots & f_{1n} \\ f_{21} & f_{22} \cdots & f_{2,n+1} \cdots & f_{2n} \\ \vdots & & \vdots & \\ f_{n1} & f_{n2} & f_{n,n+1} \cdots & f_{nn} \end{bmatrix}}{\begin{bmatrix} f_{11} & f_{12} & \cdots & f_{1n} \\ f_{21} & f_{22} & \cdots & f_{2n} \\ \vdots & & & \\ f_{n1} & f_{n2} & \cdots & f_{nn} \end{bmatrix}} \qquad n = 1, \ldots n. \tag{39}$$

EXAMPLES

In this section, two specific working examples on the prediction of concentration polarization based on the method discussed above are presented. They are:

(A) Two-Solute System

The system is assumed to consist of NaCl (designated as component 1) and KCl (component 2). The values of other parameters are:

$$B_1 = 7.4$$

$$B_2 = 0.5$$

$$r_{12} = 0.1,\ 1.0 \text{ and } 10.0$$

The Sherwood number data of component 1, $(N_{Sh})_1$, is taken to be the same as that of one-solute system for the same values of B_1 and B_2 and can be obtained from reference (3). $(N_{Sh})_2$ is estimated according to

$$(N_{Sh})_2 = (N_{Sh})_1 \frac{(N_{Sc})_2^{1/3}}{(N_{Sc})_1^{1/3}} = (N_{Sh})_1 \left(\frac{385}{560}\right)^{1/3} .$$

Based on these Sherwood number data, the wall concentrations of components 1 and 2 were calculated according to Equations (27) and (28) with the initial concentration $a_1 = 1$, $a_2 = 1$ at $x^* = 0$. The results are shown in Figures 1-3. Also presented in these figures are the results of reference (5) which give the wall concentration of the same problem by the solution of the pertinent diffusion equations. The agreement is reasonably good and the percentage error in terms of concentration polarization (i.e. $C_w^* - 1$) in all cases is less than 10%.

(B) Three-Solute System

The feed stream is considered to consist of $CaCl_2$ (component 1), NaCl (2) and KCl (3). The other parameters are:

$$B_1 = 7.40$$

$$B_2 = 0.5$$

$$r_{12} = r_{13} = 1$$

As before, $(N_{Sh})_3$ (i.e. NaCl), is taken directly from reference (3). $(N_{Sh})_1$ and $(N_{Sh})_3$ are estimated as:

$$(N_{Sh})_1 = \frac{(N_{Sc})_1^{1/3}}{(N_{Sc})_2^{1/3}} (N_{Sh})_2 = (\frac{720}{560})^{1/3} (N_{Sh})_2$$

$$(N_{Sh})_3 = \frac{(N_{Sc})_3^{1/3}}{(N_{Sc})_2^{1/3}} (N_{Sh})_2 = (\frac{385}{510})^{1/3} (N_{Sh})_2$$

Based on these data, Equation (39) is solved for m=3 and the results are shown in Figure 4. Also included in the figures are the results obtained for the direct solution of the pertinent diffusion equation, which was made in a manner similar to that described in reference (5). The accuracy is comparable with that of the previous examples of two solute cases.

Both examples demonstrate the workability of this simplified method. It should be pointed out that the basic equations [Equations (27), (28) or (39)] are exact and involve no simplifications. The discrepancy between the results from this method and those of more exact methods is entirely due to the error introduced in the estimation of the Sherwood number data. It, therefore, may be instructive to look into this more carefully. In Table 1, a comparison of the local Sherwood number corresponding to the first examples between those obtained from the exact solution and the estimated value which was used in Example A is given. The procedure suggested in this work for the estimation of the Sherwood number represents just one possibility. With ever-increasing interest in reverse osmosis as a separation process, more reliable methods for estimating Sherwood number information would undoubtedly be developed in the future through either direct experimentation or more exact analysis, which, in turn, would improve the accuracy in the use of this method for the estimation of concentration polarization.

In addition to the prediction of concentration polarization, the present method can also be used for the purpose of interpolation. For a numerical

treatment as described in references (3,4), the question of predicting the results for conditions not specifically covered in numerical calculation presents some difficulty because of the absence of closed form expression. Owing to the large number of parameters involved, only a limited number of cases can be studied and it is impractical to establish a so-called "master plot". Consequently, it is desirable to have a procedure which can predict the concentration build-up along the membrane surface based on available results. Since the Sherwood number depends much less on the system parameters than the wall concentration, it is easier to interpolate the Sherwood number. Once the Sherwood number variation is known as a function of longitudinal position, the present method may be used to calculate the wall concentration. For example, for the single solute case it can be readily shown that

$$\frac{da_1}{dx^+} = \frac{\frac{B_1 B_2 G_1^2}{(N_{Sc})_1}(a_1 - 1) - (G_1 + a_1)\frac{d}{dx^+}(N_{Sh})_1 - a}{(N_{Sh})_1\left[(N_{Sc})_1 (V_w^+) - (N_{Sh})_1\right] - B_1 B_2 f_1}$$

where

$$V_w^+ = \frac{B_1}{(N_{Sc})_1}\left[1 - B_2 f_1\right]$$

Also, assuming that the Sherwood number is proportional to the cube root of Schmidt number, the performance of a reverse osmosis system for other species of solute may also be determined.

ACKNOWLEDGMENT

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LITERATURE CITED

1. Gill, W.N., Tien, Chi, and Zeh, Dale W., Int. J. Heat and Mass Transfer, 9, 907 (1966).

2. Gill, W.N., Zeh, Dale W., and Tien, Chi, A.I.Ch.E. J. 12, 1141 (1966).

3. Srinivasan, S., Tien, Chi, and Gill, W.N., Chem. Eng. Sci., 22, 417 (1967).

4. Srinivasan, S., and Tien, Chi, Desalination, 3, 5 (1967).

5. Srinivasan, S., and Tien, Chi, "Reverse Osmosis in Multicomponent System", to be published in Desalination.

NOMENCLATURE

A	=	membrane constant
a_1	=	wall concentration of solute 1
a_j	=	wall concentration of the j^{th} species
B_2	=	$(\pi_{os})_o/\Delta P$
b	=	half the distance between the plates
C_j	=	concentration of the j^{th} solute
C_j^+	=	$C_j/(C_j)_o$
$(C_j)_o$	=	concentration of solute j at inlet
$(C_j)_b$	=	bulk concentration of solute j
$(C_j)_w$	=	wall concentration of solute j
$(C_j^+)_b$	=	$(C_j)_b/(C_j)_o$
$(C_j^+)_w$	=	$(C_j)_w/(C_j)_o$
D_{jj}	=	diffusion coefficient of solute j
f_1, f_2, f_3	=	defined by Equations (20-23)
f_{1j}	=	functions defined by Equations (38a) - (38b)
G_1, G_2	=	defined by Equations (16,17)
G_j	=	defined by Equation (36)
g_1, g_2, g_3	=	defined by Equations (24) - (26)
$(k_j)_x$	=	mass transfer coefficient of solute j
N_{Re_I}	=	bU_o/ν
$(N_{Sc})_j$	=	Schmidt number for solute j
$(N_{Sh})_j$	=	Sherwood number for solute j

NOMENCLATURE (Cont'd.)

Q	=	volumetric production per unit width
Q^+	=	fraction of water withdrawn
r_{12}	=	$(C_1)_o/(C_2)_o$
r_{13}	=	$(C_1)_o/(C_3)_o$
u	=	component of velocity in the x direction
U_o	=	average velocity at inlet
V_w	=	wall velocity
V_w^+	=	bV_w/ν
x	=	axial distance along duct
x^+	=	$x/b\ R_{e_I}$
y	=	distance normal to membrane from membrane surface
y^+	=	y/b

Greek letters

α	=	defined by Equation (3.4)
β	=	defined by Equation (3.5)
ϵ_n	=	defined by Equation (31)
γ_j	=	defined by Equation (32)
$\Delta_v p$	=	pressure drop across the membrane
	=	Kinematic Viscosity
Π	=	Osmotic Pressure
$(\Pi_{ca})_o$	=	Osmotic Pressure at Inlets.

TABLE 1

$B_1 = 7.4074 \quad B_2 = 0.5 \quad \gamma_{12} = 1$

x^+	$(N_{Sh})_1$ (Actual)	$(N_{Sh})_1$ (Single Component)	$(N_{Sh})_2$ (Actual)	$(N_{Sh})_2$ (Single Component)
0.006	58.787	58.489	54.470	51.622
0.010	47.145	46.564	43.678	41.097
0.050	24.237	23.255	22.274	20.523
0.100	18.586	17.730	17.010	15.648
0.50	11.144	10.972	10.06	9.683
1.00	8.976	8.857	8.084	7.817
5.00	5.467	5.390	4.916	4.758
10.00	4.443	4.381	4.014	3.867
15.00	3.949	3.598	3.591	3.441
20.-0	3.643	3.605	3.335	3.183

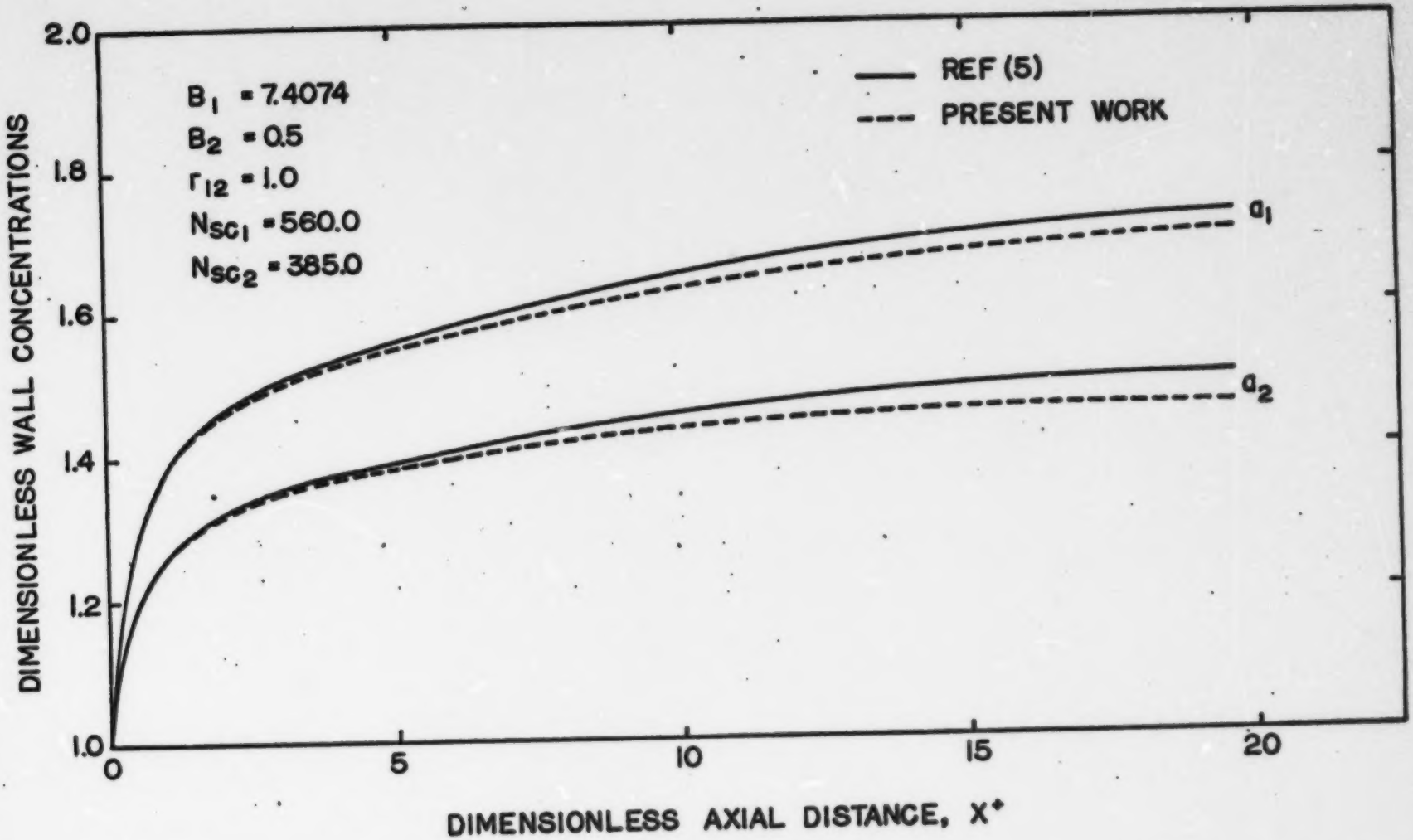

FIGURE 1. COMPARISON BETWEEN THIS METHOD AND NUMERICAL SOLUTION.

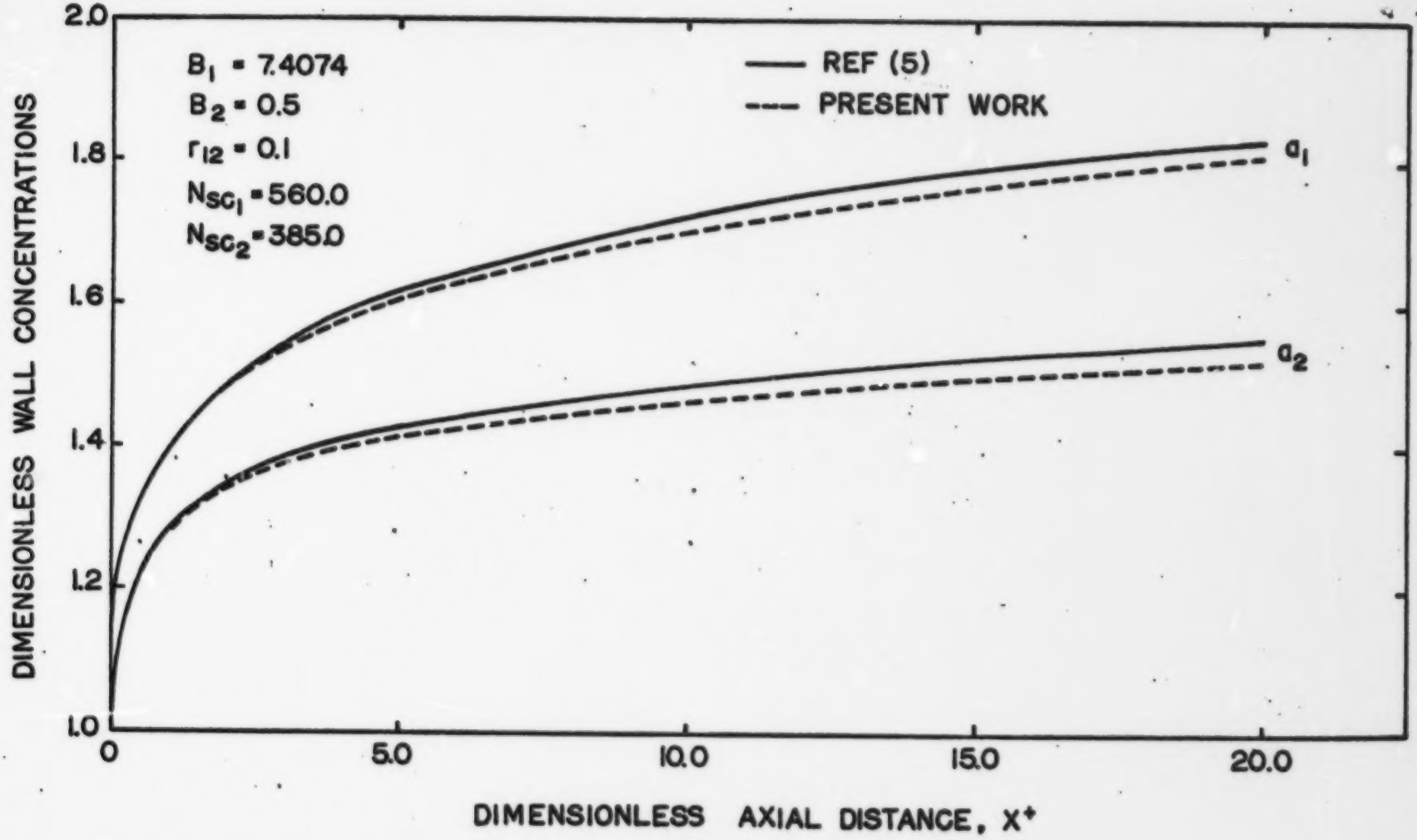

FIGURE 2. COMPARISON BETWEEN THIS METHOD AND NUMERICAL SOLUTION.

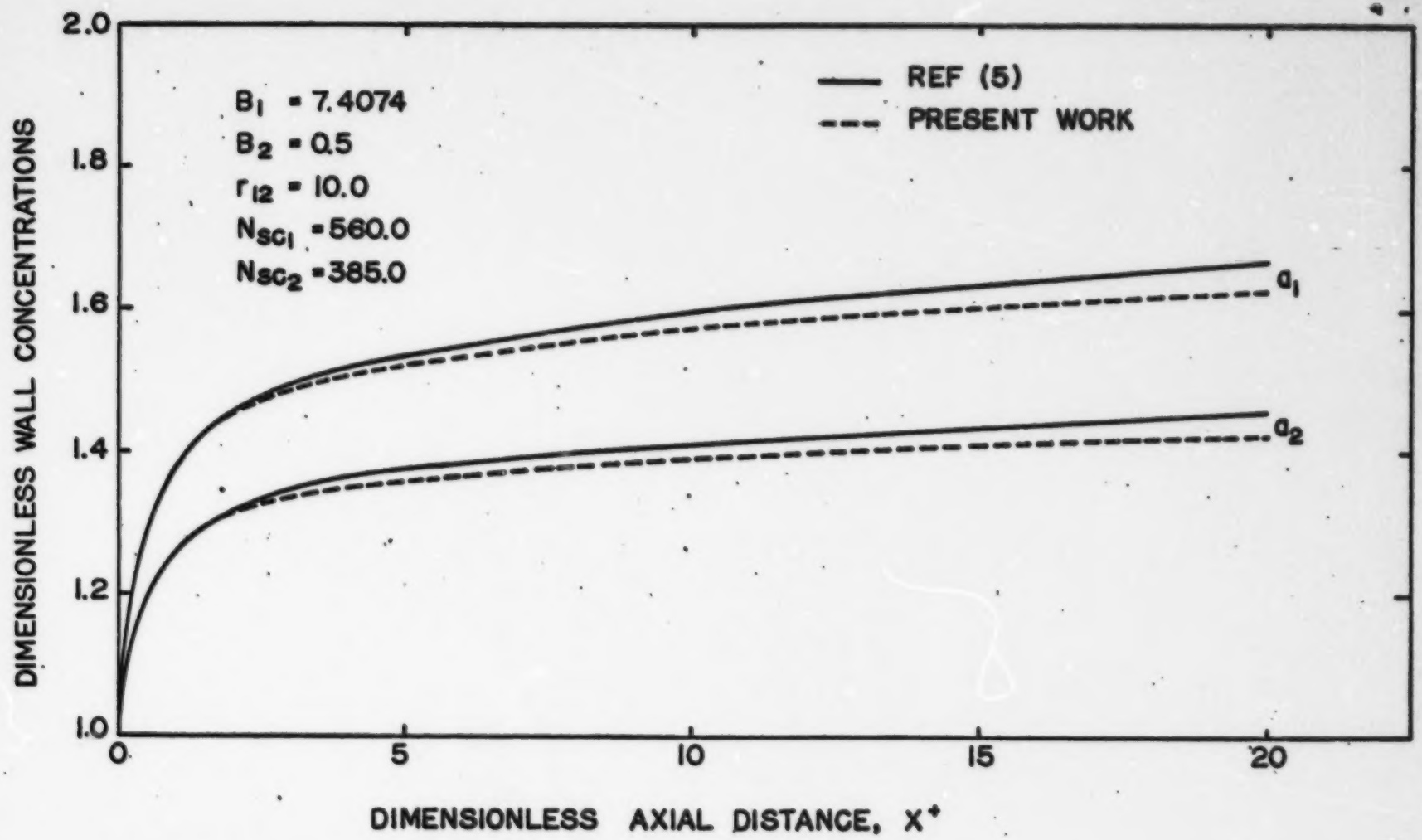

FIGURE 3. COMPARISON BETWEEN THIS METHOD AND NUMERICAL SOLUTION.

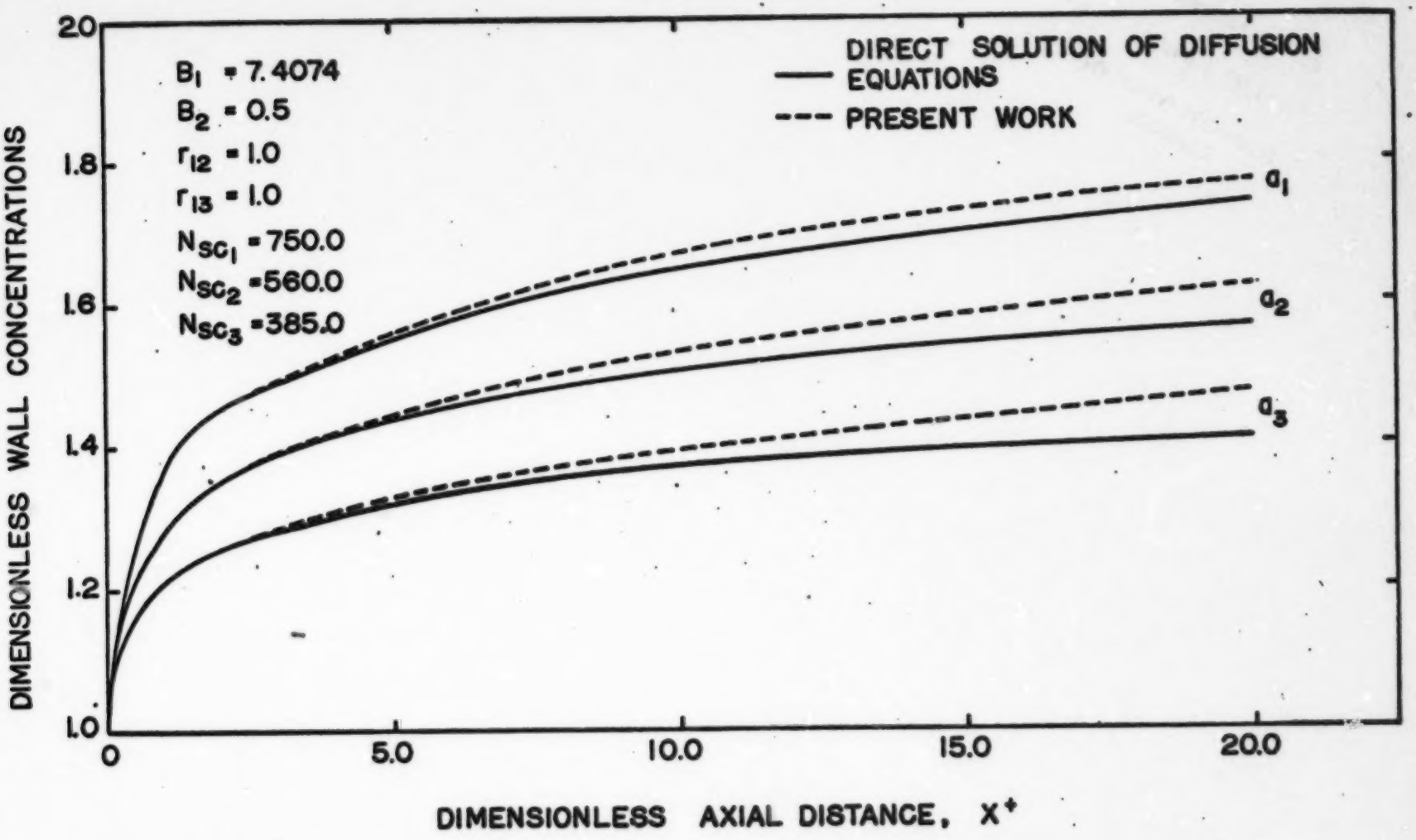

FIGURE 4. COMPARISON BETWEEN THIS METHOD AND NUMERICAL SOLUTION.